

**METHOD AND SYSTEM OF COMPUTING AND RENDERING THE NATURE OF
ATOMS AND ATOMIC IONS**

This application claims priority to U.S. Provisional Appl'n Ser. Nos.
5 60/542,278, filed February 9, 2004, and 60/534,112, filed January 5, 2004, the
complete disclosures of which are incorporated herein by reference.

This application also claims priority to U.S. Provisional Appl'n entitled "The
Grand Unified Theory of Classical Quantum Mechanics" filed January 3, 2005,
attorney docket No. 62226-BOOK1, the complete disclosure of which is incorporated
10 herein by reference.

1. Field of the Invention

This invention relates to a method and system of physically solving the
15 charge, mass, and current density functions of atoms and atomic ions and
computing and rendering the nature of these species using the solutions. The
results can be displayed on visual or graphical media. The displayed information is
useful to anticipate reactivity and physical properties, as well as for educational
purposes. The insight into the nature of bound electrons can permit the solution and
20 display of other atoms and ions and provide utility to anticipate their reactivity and
physical properties.

2. Background of the Invention

25 While it is true that the Schrödinger equation can be solved exactly for the
hydrogen atom, the result is not the exact solution of the hydrogen atom since
electron spin is missed entirely and there are many internal inconsistencies and
nonphysical consequences that do not agree with experimental results. The Dirac
equation does not reconcile this situation. Many additional shortcomings arise such
30 as instability to radiation, negative kinetic energy states, intractable infinities, virtual
particles at every point in space, the Klein paradox, violation of Einstein causality,
and "spooky" action at a distance. Despite its successes, quantum mechanics (QM)
has remained mysterious to all who have encountered it. Starting with Bohr and
progressing into the present, the departure from intuitive, physical reality has
35 widened. The connection between quantum mechanics and reality is more than just
a "philosophical" issue. It reveals that quantum mechanics is not a correct or
complete theory of the physical world and that inescapable internal inconsistencies

and incongruities arise when attempts are made to treat it as a physical as opposed to a purely mathematical "tool". Some of these issues are discussed in a review by Laloë [Reference No. 1]. But, QM has severe limitations even as a tool. Beyond one-electron atoms, multielectron-atom quantum mechanical equations can not be solved except by approximation methods involving adjustable-parameter theories (perturbation theory, variational methods, self-consistent field method, multi-configuration Hartree Fock method, multi-configuration parametric potential method, $1/Z$ expansion method, multi-configuration Dirac-Fock method, electron correlation terms, QED terms, etc.)—all of which contain assumptions that can not be physically tested and are not consistent with physical laws. In an attempt to provide some physical insight into atomic problems and starting with the same essential physics as Bohr of e^- moving in the Coulombic field of the proton and the wave equation as modified after Schrödinger, a classical approach was explored which yields a model which is remarkably accurate and provides insight into physics on the atomic level [2-4].

Physical laws and intuition are restored when dealing with the wave equation and quantum mechanical problems. Specifically, a theory of classical quantum mechanics (CQM) was derived from first principles that successfully applies physical laws on all scales. Rather than use the postulated Schrödinger boundary condition: " $\Psi \rightarrow 0$ as $r \rightarrow \infty$ ", which leads to a purely mathematical model of the electron, the constraint is based on experimental observation. Using Maxwell's equations, *the classical wave equation is solved with the constraint that the bound $n = 1$ -state electron cannot radiate energy.* The electron must be extended rather than a point. On this basis with the assumption that physical laws including Maxwell's equation apply to bound electrons, the hydrogen atom was solved exactly from first principles. The remarkable agreement across the spectrum of experimental results indicates that this is the correct model of the hydrogen atom. In the present invention, the physical approach was applied to multielectron atoms that were solved exactly disproving the deep-seated view that such exact solutions can not exist according to quantum mechanics. The general solutions for one through twenty-electron atoms are given. The predictions are in remarkable agreement with the experimental values known for 400 atoms and ions.

Classical Quantum Theory of the Atom Based on Maxwell's Equations

The old view that the electron is a zero or one-dimensional point in an all-space probability wave function $\Psi(x)$ is not taken for granted. The theory of classical quantum mechanics (CQM), derived from first principles, must successfully and consistently apply physical laws on all scales [2-7]. Historically, the point at which QM broke with classical laws can be traced to the issue of nonradiation of the one electron atom that was addressed by Bohr with a postulate of stable orbits in defiance of the physics represented by Maxwell's equations [2-9]. Later physics was replaced by "pure mathematics" based on the notion of the inexplicable wave-particle duality nature of electrons which lead to the Schrödinger equation wherein the consequences of radiation predicted by Maxwell's equations were ignored. Ironically, both Bohr and Schrödinger used the electrostatic Coulomb potential of Maxwell's equations, but abandoned the electrodynamic laws. Physical laws may indeed be the root of the observations thought to be "purely quantum mechanical", and it may have been a mistake to make the assumption that Maxwell's electrodynamic equations must be rejected at the atomic level. Thus, in the present approach, the classical wave equation is solved with the constraint that a bound $n = 1$ -state electron cannot radiate energy.

Thus, herein, derivations consider the electrodynamic effects of moving charges as well as the Coulomb potential, and the search is for a solution representative of the electron wherein there is acceleration of charge motion without radiation. The mathematical formulation for zero radiation based on Maxwell's equations follows from a derivation by Haus [16]. The function that describes the motion of the electron must not possess spacetime Fourier components that are synchronous with waves traveling at the speed of light. Similarly, nonradiation is demonstrated based on the electron's electromagnetic fields and the Poynting power vector.

It was shown previously [2-6] that CQM gives closed form solutions for the atom including the stability of the $n = 1$ state and the instability of the excited states, the equation of the photon and electron in excited states, the equation of the free electron, and photon which predict the wave particle duality behavior of particles and light. The current and charge density functions of the electron may be directly physically interpreted. For example, spin angular momentum results from the

motion of negatively charged mass moving systematically, and the equation for angular momentum, $\mathbf{r} \times \mathbf{p}$, can be applied directly to the wave function (a current density function) that describes the electron. The magnetic moment of a Bohr magneton, Stern Gerlach experiment, g factor, Lamb shift, resonant line width and shape, selection rules, correspondence principle, wave particle duality, excited states, reduced mass, rotational energies, and momenta, orbital and spin splitting, spin-orbital coupling, Knight shift, and spin-nuclear coupling, and elastic electron scattering from helium atoms, are derived in closed form equations based on Maxwell's equations. The calculations agree with experimental observations. In contrast to the failure of the Bohr theory and the nonphysical, adjustable-parameter approach of quantum mechanics, the nature of the chemical bond is given in exact solutions of hydrogen molecular ions and molecules that match the data for 26 parameters [3]. In another published article, rather than invoking renormalization, untestable virtual particles, and polarization of the vacuum by the virtual particles, the results of QED such as the anomalous magnetic moment of the electron, the Lamb Shift, the fine structure and hyperfine structure of the hydrogen atom, and the hyperfine structure intervals of positronium and muonium (thought to be only solvable using QED) are solved exactly from Maxwell's equations to the limit possible based on experimental measurements [6].

In contrast to short comings of quantum mechanical equations, with CQM, multielectron atoms can be exactly solved in closed form. Using the nonradiative wave equation solutions that describe the bound electron having conserved momentum and energy, the radii are determined from the force balance of the electric, magnetic, and centrifugal forces that corresponds to the minimum of energy of the system. The ionization energies are then given by the electric and magnetic energies at these radii. One through twenty-electron atoms are solved exactly except for nuclear hyperfine structure effects of atoms other than hydrogen. (The spreadsheets to calculate the energies are available from the internet [17]). For 400 atoms and ions the agreement between the predicted and experimental results are remarkable.

Using the same unique physical model for the two-electron atom in all cases, it was confirmed that the CQM solutions give the accurate model of atoms and ions by solving conjugate parameters of the free electron, ionization energy of helium and all two electron atoms, electron scattering of helium for all angles, and all He I

excited states as well as the ionization energies of multielectron atoms provided herein. Over five hundred conjugate parameters are calculated using a unique solution of the two-electron atom without any adjustable parameters to achieve overall agreement to the level obtainable considering the error in the measurements
5 and the fundamental constants in the closed-form equations [5].

The background theory of classical quantum mechanics (CQM) for the physical solutions of atoms and atomic ions is disclosed in R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, January 2000 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '00 Mills GUT"), provided by BlackLight
10 Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, September 2001 Edition, BlackLight Power, Inc., Cranbury, New Jersey, Distributed by Amazon.com (" '01 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*,
15 July 2004 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '04 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512; R. Mills, *The Grand Unified Theory of Classical Quantum Mechanics*, January 2005 Edition, BlackLight Power, Inc., Cranbury, New Jersey, (" '05 Mills GUT"), provided by BlackLight Power, Inc., 493 Old Trenton Road, Cranbury, NJ, 08512 (posted at
20 www.blacklightpower.com and filed as a U.S. Provisional Application on January 3, 2005, entitled "The Grand Unified Theory of Classical Quantum Mechanics," attorney docket No. 62226-BOOK1); in prior PCT applications PCT/US02/35872; PCT/US02/06945; PCT/US02/06955; PCT/US01/09055; PCT/US01/ 25954; PCT/US00/20820; PCT/US00/20819; PCT/US00/09055; PCT/US99/17171;
25 PCT/US99/17129; PCT/US 98/22822; PCT/US98/14029; PCT/US96/07949; PCT/US94/02219; PCT/US91/08496; PCT/US90/01998; and PCT/US89/05037 and U.S. Patent No. 6,024,935; the entire disclosures of which are all incorporated herein by reference; (hereinafter "Mills Prior Publications").

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SUMMARY OF THE INVENTION

An object of the present invention is to solve the charge (mass) and current-density functions of atoms and atomic ions from first principles. In an embodiment, the solution is derived from Maxwell's equations invoking the constraint that the
35 bound electron does not radiate even though it undergoes acceleration.

Another objective of the present invention is to generate a readout, display, image, or other output of the solutions so that the nature of atoms and atomic ions can be better understood and applied to predict reactivity and physical properties of atoms, ions and compounds.

- 5 Another objective of the present invention is to apply the methods and systems of solving the nature of bound electrons and its rendering to numerical or graphical form to all atoms and atomic ions.

These objectives and other objectives are met by a system of computing and rendering the nature of bound atomic and atomic ionic electrons from physical
10 solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, comprising:

processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in a selected atom or ion, wherein the
15 equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

a display in communication with the processing means for displaying the current and charge density representation of the electron(s) of the selected atom or ion.

- 20 These objectives and other objectives are also met by a system of computing the nature of bound atomic and atomic ionic electrons from physical solutions of the charge, mass, and current density functions of atoms and atomic ions, which solutions are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration, comprising:

25 processing means for processing and solving the equations for charge, mass, and current density functions of electron(s) in selected atoms or ions, wherein the equations are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration; and

output means for outputting the solutions of the charge, mass, and current
30 density functions of the atoms and atomic ions.

These objectives and other objectives are further met by a method comprising the steps of;

a.) inputting electron functions that are derived from Maxwell's equations using a constraint that the bound electron(s) does not radiate under acceleration;

- b.) inputting a trial electron configuration;
- c.) inputting the corresponding centrifugal, Coulombic, diamagnetic and paramagnetic forces,
- d.) forming the force balance equation comprising the centrifugal force equal
- 5 to the sum of the Coulombic, diamagnetic and paramagnetic forces;
- e.) solving the force balance equation for the electron radii;
- f.) calculating the energy of the electrons using the radii and the corresponding electric and magnetic energies;
- g.) repeating Steps a-f for all possible electron configurations, and
- 10 h.) outputting the lowest energy configuration and the corresponding electron radii for that configuration.

The invention will now be described with reference to classical quantum mechanics. A theory of classical quantum mechanics (CQM) was derived from first principles that successfully applies physical laws on all scales [2-6], and the

15 mathematical connection with the Schrödinger equation to relate it to physical laws was discussed previously [27]. The physical approach based on Maxwell's equations was applied to multielectron atoms that were solved exactly. The classical predictions of the ionization energies were solved for the physical electrons comprising concentric orbitspheres ("bubble-like" charge-density functions) that are

20 electrostatic and magnetostatic corresponding to a constant charge distribution and a constant current corresponding to spin angular momentum. Alternatively, the charge is a superposition of a constant and a dynamical component. In the latter case, charge density waves on the surface are time and spherically harmonic and correspond additionally to electron orbital angular momentum that superimposes the

25 spin angular momentum. Thus, the electrons of multielectron atoms all exist as orbitspheres of discrete radii which are given by r_n of the radial Dirac delta function, $\delta(r - r_n)$. These electron orbitspheres may be spin paired or unpaired depending on the force balance which applies to each electron. Ultimately, the electron configuration must be a minimum of energy. Minimum energy configurations are

30 given by solutions to Laplace's equation. As demonstrated previously, this general solution also gives the functions of the resonant photons of excited states [4]. It was found that electrons of an atom with the same principal and ℓ quantum numbers align parallel until each of the m_ℓ levels are occupied, and then pairing occurs until

each of the m_l levels contain paired electrons. The electron configuration for one through twenty-electron atoms that achieves an energy minimum is: $1s < 2s < 2p < 3s < 3p < 4s$. In each case, the corresponding force balance of the central Coulombic, paramagnetic, and diamagnetic forces was derived for each n -electron atom that was solved for the radius of each electron. The central Coulombic force was that of a point charge at the origin since the electron charge-density functions are spherically symmetrical with a time dependence that was nonradiative. This feature eliminated the electron-electron repulsion terms and the intractable infinities of quantum mechanics and permitted general solutions. The ionization energies were obtained using the calculated radii in the determination of the Coulombic and any magnetic energies. The radii and ionization energies for all cases were given by equations having fundamental constants and each nuclear charge, Z , only. The predicted ionization energies and electron configurations given in TABLES I-XXIII are in remarkable agreement with the experimental values known for 400 atoms and ions.

The presented exact physical solutions for the atom and all ions having a given number of electrons can be used to predict the properties of elements and engineer compositions of matter in a manner which is not possible using quantum mechanics.

In an embodiment., the physical, Maxwellian solutions for the dimensions and energies of atom and atomic ions are processed with a processing means to produce an output. Embodiments of the system for performing computing and rendering of the nature of the bound atomic and atomic-ionic electrons using the physical solutions may comprise a general purpose computer. Such a general purpose computer may have any number of basic configurations. For example, such a general purpose computer may comprise a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or other storage device, an input means such as a keyboard or mouse, a display device, and a printer or other output device. A system implementing the present invention can also comprise a special purpose computer or other hardware system and all should be included within its scope.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 shows the orbitsphere in accordance with the present invention

that is a two dimensional spherical shell of zero thickness with the Bohr radius of the hydrogen atom, $r = a_H$.

FIGURE 2 shows the current pattern of the orbitsphere in accordance with the present invention from the perspective of looking along the z-axis. The current and charge density are confined to two dimensions at $r_n = nr_1$. The corresponding charge density function is uniform.

FIGURE 3 shows that the orbital function modulates the constant (spin) function (shown for $t = 0$; three-dimensional view).

FIGURE 4 shows the normalized radius as a function of the velocity due to relativistic contraction, and

FIGURE 5 shows the magnetic field of an electron orbitsphere (z-axis defined as the vertical axis).

DETAILED DESCRIPTION OF THE INVENTION

The following preferred embodiments of the invention disclose numerous calculations which are merely intended as illustrative examples. Based on the detailed written description, one skilled in the art would easily be able to practice this invention within other like calculations to produce the desired result without undue effort.

ONE-ELECTRON ATOMS

One-electron atoms include the hydrogen atom, He^+ , Li^{2+} , Be^{3+} , and so on. The mass-energy and angular momentum of the electron are constant; this requires that the equation of motion of the electron be temporally and spatially harmonic. Thus, the classical wave equation applies and

$$\left[\nabla^2 - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right] \rho(r, \theta, \phi, t) = 0 \quad (1)$$

where $\rho(r, \theta, \phi, t)$ is the time dependent charge density function of the electron in time and space. In general, the wave equation has an infinite number of solutions. To arrive at the solution which represents the electron, a suitable boundary condition must be imposed. It is well known from experiments that each single atomic electron of a given isotope radiates to the same stable state. Thus, the physical boundary condition of nonradiation of the bound electron was imposed on the solution of the wave equation for the time dependent charge density function of the

electron [2, 4]. The condition for radiation by a moving point charge given by Haus [16] is that its spacetime Fourier transform does possess components that are synchronous with waves traveling at the speed of light. Conversely, it is proposed that the condition for nonradiation by an ensemble of moving point charges that
 5 comprises a current density function is

For non-radiative states, the current-density function must NOT possess spacetime Fourier components that are synchronous with waves traveling at the speed of light.

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The time, radial, and angular solutions of the wave equation are separable. The motion is time harmonic with frequency ω_n . A constant angular function is a solution to the wave equation. Solutions of the Schrödinger wave equation comprising a radial function radiate according to Maxwell's equation as shown previously by
 15 application of Haus' condition [4]. In fact, it was found that any function which permitted radial motion gave rise to radiation. A radial function which does satisfy the boundary condition is a radial delta function

$$f(r) = \frac{1}{r^2} \delta(r - r_n) \quad (2)$$

This function defines a constant charge density on a spherical shell where $r_n = nr_1$
 20 wherein n is an integer in an excited state, and Eq. (1) becomes the two-dimensional wave equation plus time with separable time and angular functions. Given time harmonic motion and a radial delta function, the relationship between an allowed radius and the electron wavelength is given by

$$2\pi r_n = \lambda_n \quad (3)$$

25 where the integer subscript n here and in Eq. (2) is determined during photon absorption as given in the Excited States of the One-Electron Atom (Quantization) section of Ref. [4]. Using the observed de Broglie relationship for the electron mass where the coordinates are spherical,

$$\lambda_n = \frac{h}{p_n} = \frac{h}{m_e v_n} \quad (4)$$

30 and the magnitude of the velocity for every point on the orbitsphere is

$$v_n = \frac{\hbar}{m_e r_n} \quad (5)$$

The sum of the $|L_i|$, the magnitude of the angular momentum of each infinitesimal point of the orbitsphere of mass m_i , must be constant. The constant is \hbar .

$$\sum |L_i| = \sum |\mathbf{r} \times m_i \mathbf{v}| = m_e r_n \frac{\hbar}{m_e r_n} = \hbar \quad (6)$$

Thus, an electron is a spinning, two-dimensional spherical surface (zero thickness), called an *electron orbitsphere* shown in Figure 1, that can exist in a bound state at only specified distances from the nucleus determined by an energy minimum. The corresponding current function shown in Figure 2 which gives rise to the phenomenon of *spin* is derived in the Spin Function section. (See the Orbitsphere Equation of Motion for $\ell = 0$ of Ref. [4] at Chp. 1.)

Nonconstant functions are also solutions for the angular functions. To be a harmonic solution of the wave equation in spherical coordinates, these angular functions must be spherical harmonic functions [18]. A zero of the spacetime Fourier transform of the product function of two spherical harmonic angular functions, a time harmonic function, and an unknown radial function is sought. The solution for the radial function which satisfies the boundary condition is also a delta function given by Eq. (2). Thus, bound electrons are described by a charge-density (mass-density) function which is the product of a radial delta function, two angular functions (spherical harmonic functions), and a time harmonic function.

$$\rho(r, \theta, \phi, t) = f(r) A(\theta, \phi, t) = \frac{1}{r^2} \delta(r - r_n) A(\theta, \phi, t); \quad A(\theta, \phi, t) = Y(\theta, \phi) k(t) \quad (7)$$

In these cases, the spherical harmonic functions correspond to a traveling charge density wave confined to the spherical shell which gives rise to the phenomenon of orbital angular momentum. The orbital functions which modulate the constant "spin" function shown graphically in Figure 3 are given in the Angular Functions section.

SPIN FUNCTION

The orbitsphere spin function comprises a constant charge (current) density function with moving charge confined to a two-dimensional spherical shell. The magnetostatic current pattern of the orbitsphere spin function comprises an infinite series of correlated orthogonal great circle current loops wherein each point charge (current) density element moves time harmonically with constant angular velocity

$$\omega_n = \frac{\hbar}{m_e r_n^2} \quad (8)$$

The uniform current density function $Y_0^0(\phi, \theta)$, the orbitsphere equation of motion of the electron (Eqs. (13-14)), corresponding to the constant charge function of the orbitsphere that gives rise to the spin of the electron is generated from a basis set current-vector field defined as the orbitsphere current-vector field ("orbitsphere-cvf"). This in turn is generated over the surface by two complementary steps of an infinite series of nested rotations of two orthogonal great circle current loops where the coordinate axes rotate with the two orthogonal great circles that serve as a basis set. The algorithm to generate the current density function rotates the great circles and the corresponding $x'y'z'$ coordinates relative to the xyz frame. Each infinitesimal rotation of the infinite series is about the new i' -axis and new j' -axis which results from the preceding such rotation. Each element of the current density function is obtained with each conjugate set of rotations. In Appendix III of Ref. [4], the *continuous* uniform electron current density function $Y_0^0(\phi, \theta)$ having the same angular momentum components as that of the orbitsphere-cvf is then exactly generated from this orbitsphere-cvf as a basis element by a convolution operator comprising an autocorrelation-type function.

For Step One, the current density elements move counter clockwise on the great circle in the $y'z'$ -plane and move clockwise on the great circle in the $x'z'$ -plane. The great circles are rotated by an infinitesimal angle $\pm\Delta\alpha$, (a positive rotation around the x' -axis or a negative rotation about the z' -axis for Steps One and Two, respectively) and then by $\pm\Delta\alpha$, (a positive rotation around the new y' -axis or a positive rotation about the new x' -axis for Steps One and Two, respectively). The coordinates of each point on each rotated great circle (x', y', z') is expressed in terms of the first (x, y, z) coordinates by the following transforms where clockwise rotations and motions are defined as positive looking along the corresponding axis:

Step One

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cos(\Delta\alpha_y) & 0 & -\sin(\Delta\alpha_y) \\ 0 & 1 & 0 \\ \sin(\Delta\alpha_y) & 0 & \cos(\Delta\alpha_y) \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\Delta\alpha_x) & \sin(\Delta\alpha_x) \\ 0 & -\sin(\Delta\alpha_x) & \cos(\Delta\alpha_x) \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cos(\Delta\alpha_y) & \sin(\Delta\alpha_y)\sin(\Delta\alpha_x) & -\sin(\Delta\alpha_y)\cos(\Delta\alpha_x) \\ 0 & \cos(\Delta\alpha_x) & \sin(\Delta\alpha_x) \\ \sin(\Delta\alpha_y) & -\cos(\Delta\alpha_y)\sin(\Delta\alpha_x) & \cos(\Delta\alpha_y)\cos(\Delta\alpha_x) \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad (9)$$

5 Step Two

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\Delta\alpha_x) & \sin(\Delta\alpha_x) \\ 0 & -\sin(\Delta\alpha_x) & \cos(\Delta\alpha_x) \end{bmatrix} \begin{bmatrix} \cos(\Delta\alpha_z) & \sin(\Delta\alpha_z) & 0 \\ -\sin(\Delta\alpha_z) & \cos(\Delta\alpha_z) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cos(\Delta\alpha_z) & \sin(\Delta\alpha_z) & 0 \\ -\cos(\Delta\alpha_x)\sin(\Delta\alpha_z) & \cos(\Delta\alpha_x)\cos(\Delta\alpha_z) & \sin(\Delta\alpha_x) \\ \sin(\Delta\alpha_x)\sin(\Delta\alpha_z) & -\sin(\Delta\alpha_x)\cos(\Delta\alpha_z) & \cos(\Delta\alpha_x) \end{bmatrix} \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad (10)$$

where the angular sum is $\lim_{\Delta\alpha \rightarrow 0} \sum_{n=1}^{\frac{\sqrt{2}}{2}\pi} |\Delta\alpha_{i,j}| = \frac{\sqrt{2}}{2}\pi$.

The orbitsphere-cvf is given by n reiterations of Eqs. (9) and (10) for each point on each of the two orthogonal great circles during each of Steps One and Two. The output given by the non-primed coordinates is the input of the next iteration corresponding to each successive nested rotation by the infinitesimal angle $\pm\Delta\alpha_i$ or $\pm\Delta\alpha_j$, where the magnitude of the angular sum of the n rotations about each of the i' -axis and the j' -axis is $\frac{\sqrt{2}}{2}\pi$. Half of the orbitsphere-cvf is generated during each of

15 Steps One and Two.

Following Step Two, in order to match the boundary condition that the magnitude of the velocity at any given point on the surface is given by Eq. (5), the output half of the orbitsphere-cvf is rotated clockwise by an angle of $\frac{\pi}{4}$ about the z-axis. Using Eq. (10) with $\Delta\alpha_x = \frac{\pi}{4}$ and $\Delta\alpha_y = 0$ gives the rotation. Then, the one

- 5 half of the orbitsphere-cvf generated from Step One is superimposed with the complementary half obtained from Step Two following its rotation about the z-axis of $\frac{\pi}{4}$ to give the basis function to generate $Y_0^0(\phi, \theta)$, the orbitsphere equation of motion of the electron.

- The current pattern of the orbitsphere-cvf generated by the nested rotations
 10 of the orthogonal great circle current loops is a continuous and total coverage of the spherical surface, but it is shown as a visual representation using 6 degree increments of the infinitesimal angular variable $\pm\Delta\alpha_i$ and $\pm\Delta\alpha_j$ of Eqs. (9) and (10) from the perspective of the z-axis in Figure 2. In each case, the complete orbitsphere-cvf current pattern corresponds all the orthogonal-great-circle elements
 15 which are generated by the rotation of the basis-set according to Eqs. (9) and (10) where $\pm\Delta\alpha_i$ and $\pm\Delta\alpha_j$ approach zero and the summation of the infinitesimal angular rotations of $\pm\Delta\alpha_i$ and $\pm\Delta\alpha_j$ about the successive i'-axes and j'-axes is $\frac{\sqrt{2}}{2}\pi$ for each Step. The current pattern gives rise to the phenomenon corresponding to the spin quantum number. The details of the derivation of the spin
 20 function are given in Ref. [2] and Chp. 1 of Ref. [4].

- The resultant angular momentum projections of $L_{xy} = \frac{\hbar}{4}$ and $L_z = \frac{\hbar}{2}$ meet the boundary condition for the unique current having an angular velocity magnitude at each point on the surface given by Eq. (5) and give rise to the Stern Gerlach experiment as shown in Ref. [4]. The further constraint that the current density is
 25 uniform such that the charge density is uniform, corresponding to an equipotential, minimum energy surface is satisfied by using the orbitsphere-cvf as a basis element to generate $Y_0^0(\phi, \theta)$ using a convolution operator comprising an autocorrelation-type function as given in Appendix III of Ref. [4]. The operator comprises the convolution of each great circle current loop of the orbitsphere-cvf designated as the
 30 primary orbitsphere-cvf with a second orbitsphere-cvf designated as the secondary

orbitsphere-cvf wherein the convolved secondary elements are matched for orientation, angular momentum, and phase to those of the primary. The resulting exact uniform current distribution obtained from the convolution has the same angular momentum distribution, resultant, L_R , and components of $L_{xy} = \frac{\hbar}{4}$ and

- 5 $L_z = \frac{\hbar}{2}$ as those of the orbitsphere-cvf used as a primary basis element.

ANGULAR FUNCTIONS

The time, radial, and angular solutions of the wave equation are separable.

- 10 Also based on the radial solution, the angular charge and current-density functions of the electron, $A(\theta, \phi, t)$, must be a solution of the wave equation in two dimensions (plus time),

$$\left[\nabla^2 - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right] A(\theta, \phi, t) = 0 \quad (11)$$

where $\rho(r, \theta, \phi, t) = f(r)A(\theta, \phi, t) = \frac{1}{r^2} \delta(r - r_n)A(\theta, \phi, t)$ and $A(\theta, \phi, t) = Y(\theta, \phi)k(t)$

$$15 \quad \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2}{\partial \phi^2} \right) - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right] A(\theta, \phi, t) = 0 \quad (12)$$

where v is the linear velocity of the electron. The charge-density functions including the time-function factor are

$$l = 0$$

20

$$\rho(r, \theta, \phi, t) = \frac{e}{8\pi r^2} [\delta(r - r_n)] [Y_0^0(\theta, \phi) + Y_l^m(\theta, \phi)] \quad (13)$$

$$l \neq 0$$

25

$$\rho(r, \theta, \phi, t) = \frac{e}{4\pi r^2} [\delta(r - r_n)] [Y_0^0(\theta, \phi) + \text{Re} \{ Y_l^m(\theta, \phi) e^{i\omega_n t} \}] \quad (14)$$

where $Y_l^m(\theta, \phi)$ are the spherical harmonic functions that spin about the z-axis with angular frequency ω_n with $Y_0^0(\theta, \phi)$ the constant function.

$\text{Re} \{ Y_l^m(\theta, \phi) e^{i\omega_n t} \} = P_l^m(\cos \theta) \cos(m\phi + \omega_n t)$ where to keep the form of the spherical

- 30 harmonic as a traveling wave about the z-axis, $\omega_n = m\omega_n$.

ACCELERATION WITHOUT RADIATION

Special Relativistic Correction to the Electron Radius

5 The relationship between the electron wavelength and its radius is given by Eq. (3) where λ is the de Broglie wavelength. For each current density element of the spin function, the distance along each great circle in the direction of instantaneous motion undergoes length contraction and time dilation. Using a phase matching condition, the wavelengths of the electron and laboratory inertial
10 frames are equated, and the corrected radius is given by

$$r_n = r_n' \left[\sqrt{1 - \left(\frac{v}{c}\right)^2} \sin \left[\frac{\pi}{2} \left(1 - \left(\frac{v}{c}\right)^2 \right)^{3/2} \right] + \frac{1}{2\pi} \cos \left[\frac{\pi}{2} \left(1 - \left(\frac{v}{c}\right)^2 \right)^{3/2} \right] \right] \quad (15)$$

where the electron velocity is given by Eq. (5). (See Ref. [4] Chp. 1, Special Relativistic Correction to the Ionization Energies section). $\frac{e}{m_e}$ of the electron, the electron angular momentum of \hbar , and μ_B are invariant, but the mass and charge
15 densities increase in the laboratory frame due to the relativistically contracted electron radius. As $v \rightarrow c$, $r/r' \rightarrow \frac{1}{2\pi}$ and $r = \lambda$ as shown in Figure 4.

Nonradiation Based on the Spacetime Fourier Transform of the Electron Current

20 Although an accelerated *point* particle radiates, an *extended distribution* modeled as a superposition of accelerating charges does not have to radiate [14, 16, 19-21]. The Fourier transform of the electron charge density function given by Eq. (7) is a solution of the three-dimensional wave equation in frequency space (\mathbf{k}, ω space) as given in Chp 1, Spacetime Fourier Transform of the Electron Function
25 section, of Ref. [4]. Then the corresponding Fourier transform of the current density function $K(s, \Theta, \Phi, \omega)$ is given by multiplying by the constant angular frequency.

$$\begin{aligned}
K(s, \Theta, \Phi, \omega) &= 4\pi\omega_n \frac{\sin(2s_n r_n)}{2s_n r_n} \\
&\otimes 2\pi \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu-1} (\pi \sin \Theta)^{2(\nu-1)}}{(\nu-1)!(\nu-1)!} \frac{\Gamma\left(\frac{1}{2}\right) \Gamma\left(\nu + \frac{1}{2}\right)}{(\pi \cos \Theta)^{2\nu+1} 2^{\nu+1}} \frac{2\nu!}{(\nu-1)!} s^{-2\nu} \\
&\otimes 2\pi \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu-1} (\pi \sin \Phi)^{2(\nu-1)}}{(\nu-1)!(\nu-1)!} \frac{\Gamma\left(\frac{1}{2}\right) \Gamma\left(\nu + \frac{1}{2}\right)}{(\pi \cos \Phi)^{2\nu+1} 2^{\nu+1}} \frac{2\nu!}{(\nu-1)!} s^{-2\nu} \\
&\frac{1}{4\pi} [\delta(\omega - \omega_n) + \delta(\omega + \omega_n)]
\end{aligned} \tag{16}$$

$\mathbf{s}_n \cdot \mathbf{v}_n = \mathbf{s}_n \cdot \mathbf{c} = \omega_n$ implies $r_n = \lambda_n$ which is given by Eq. (15) in the case that k is the lightlike k^0 . In this case, Eq. (16) vanishes. Consequently, spacetime harmonics of

$\frac{\omega_n}{c} = k$ or $\frac{\omega_n}{c} \sqrt{\frac{\epsilon}{\epsilon_0}} = k$ for which the Fourier transform of the current-density function

5 is nonzero do not exist. Radiation due to charge motion does not occur in any medium when this boundary condition is met. Nonradiation is also determined from the fields based on Maxwell's equations as given in the Nonradiation Based on the Electromagnetic Fields and the Poynting Power Vector section *infra*.

10 Nonradiation Based on the Electron Electromagnetic Fields and the Poynting Power Vector

A point charge undergoing periodic motion accelerates and as a consequence radiates according to the Larmor formula:

$$15 \quad P = \frac{1}{4\pi\epsilon_0} \frac{2e^2}{3c^3} a^2 \tag{17}$$

where e is the charge, a is its acceleration, ϵ_0 is the permittivity of free space, and c is the speed of light. Although an accelerated *point* particle radiates, an *extended distribution* modeled as a superposition of accelerating charges does not have to radiate [14, 16, 19-21]. In Ref. [2] and Appendix I, Chp. 1 of Ref. [4], the

20 electromagnetic far field is determined from the current distribution in order to obtain the condition, if it exists, that the electron current distribution must satisfy such that the electron does not radiate. The current follows from Eqs. (13-14). The currents corresponding to Eq. (13) and first term of Eq. (14) are static. Thus, they are trivially nonradiative. The current due to the time dependent term of Eq. (14) corresponding
25 to p, d, f, etc. orbitals is

$$\begin{aligned}
\mathbf{J} &= \frac{\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N[\delta(r - r_n)] \text{Re}\{Y_\ell^m(\theta, \phi)\} [\mathbf{u}(t) \times \mathbf{r}] \\
&= \frac{\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N[\delta(r - r_n)] (P_\ell^m(\cos \theta) \cos(m\phi + \omega_n t)) [\mathbf{u} \times \mathbf{r}] \\
&= \frac{\omega_n}{2\pi} \frac{e}{4\pi r_n^2} N[\delta(r - r_n)] (P_\ell^m(\cos \theta) \cos(m\phi + \omega_n t)) \sin \theta \hat{\phi}
\end{aligned} \tag{18}$$

where to keep the form of the spherical harmonic as a traveling wave about the z-axis, $\omega_n = m\omega_n$ and N and N' are normalization constants. The vectors are defined as

$$5 \quad \hat{\phi} = \frac{\hat{\mathbf{u}} \times \hat{\mathbf{r}}}{|\hat{\mathbf{u}} \times \hat{\mathbf{r}}|} = \frac{\hat{\mathbf{u}} \times \hat{\mathbf{r}}}{\sin \theta}; \quad \hat{\mathbf{u}} = \hat{\mathbf{z}} = \text{orbital axis} \tag{19}$$

$$\hat{\theta} = \hat{\phi} \times \hat{\mathbf{r}} \tag{20}$$

"^" denotes the unit vectors $\hat{\mathbf{u}} \equiv \frac{\mathbf{u}}{|\mathbf{u}|}$, non-unit vectors are designed in bold, and the

current function is normalized. For the electron source current given by Eq. (18), each comprising a multipole of order (ℓ, m) with a time dependence $e^{i\omega_n t}$, the far-field

10 solutions to Maxwell's equations are given by

$$\mathbf{B} = -\frac{i}{k} a_M(\ell, m) \nabla \times g_\ell(kr) \mathbf{X}_{\ell, m} \tag{21}$$

$$\mathbf{E} = a_M(\ell, m) g_\ell(kr) \mathbf{X}_{\ell, m}$$

and the time-averaged power radiated per solid angle $\frac{dP(\ell, m)}{d\Omega}$ is

$$\frac{dP(\ell, m)}{d\Omega} = \frac{c}{8\pi k^2} |a_M(\ell, m)|^2 |\mathbf{X}_{\ell, m}|^2 \tag{22}$$

where $a_M(\ell, m)$ is

$$15 \quad a_M(\ell, m) = \frac{-ek^2}{c\sqrt{\ell(\ell+1)}} \frac{\omega_n}{2\pi} N_{j_\ell}(kr_n) \Theta \sin(mks) \tag{23}$$

In the case that k is the lightlike k^0 , then $k = \omega_n / c$, in Eq. (23), and Eqs. (21-22) vanishes for

$$s = vT_n = R = r_n = \lambda_n \tag{24}$$

There is no radiation.

20

MAGNETIC FIELD EQUATIONS OF THE ELECTRON

The orbitsphere is a shell of negative charge current comprising correlated charge motion along great circles. For $\ell = 0$, the orbitsphere gives rise to a magnetic moment of 1 Bohr magneton [22]. (The details of the derivation of the magnetic parameters including the electron g factor are given in Ref. [2] and Chp. 1 of Ref. [4].)

$$\mu_B = \frac{e\hbar}{2m_e} = 9.274 \times 10^{-24} \text{ JT}^{-1} \quad (25)$$

The magnetic field of the electron shown in Figure 5 is given by

$$\mathbf{H} = \frac{e\hbar}{m_e r_n^3} (\mathbf{i}_r \cos \theta - \mathbf{i}_\theta \sin \theta) \quad \text{for } r < r_n \quad (26)$$

$$\mathbf{H} = \frac{e\hbar}{2m_e r^3} (\mathbf{i}_r 2 \cos \theta + \mathbf{i}_\theta \sin \theta) \quad \text{for } r > r_n \quad (27)$$

- 5 The energy stored in the magnetic field of the electron is

$$E_{\text{mag}} = \frac{1}{2} \mu_0 \int_0^{2\pi} \int_0^\pi \int_0^\infty H^2 r^2 \sin \theta dr d\theta d\Phi \quad (28)$$

$$E_{\text{mag total}} = \frac{\pi \mu_0 e^2 \hbar^2}{m_e^2 r_1^3} \quad (29)$$

STERN-GERLACH EXPERIMENT

10

The Stern-Gerlach experiment implies a magnetic moment of one Bohr magneton and an associated angular momentum quantum number of 1/2.

Historically, this quantum number is called the spin quantum number, s

($s = \frac{1}{2}$; $m_s = \pm \frac{1}{2}$). The superposition of the vector projection of the orbitsphere

- 15 angular momentum on the z-axis is $\frac{\hbar}{2}$ with an orthogonal component of $\frac{\hbar}{4}$.

Excitation of a resonant Larmor precession gives rise to \hbar on an axis S that precesses about the z-axis called the spin axis at the Larmor frequency at an angle

of $\theta = \frac{\pi}{3}$ to give a perpendicular projection of

$$S_\perp = \pm \sqrt{\frac{3}{4}} \hbar \quad (30)$$

- 20 and a projection onto the axis of the applied magnetic field of

$$S_\parallel = \pm \frac{\hbar}{2} \quad (31)$$

The superposition of the $\frac{\hbar}{2}$, z-axis component of the orbitsphere angular momentum and the $\frac{\hbar}{2}$, z-axis component of S gives \hbar corresponding to the observed electron magnetic moment of a Bohr magneton, μ_B .

25

ELECTRON g FACTOR

Conservation of angular momentum of the orbitsphere permits a discrete change of its "kinetic angular momentum" ($\mathbf{r} \times m\mathbf{v}$) by the applied magnetic field of

- 30 $\frac{\hbar}{2}$, and concomitantly the "potential angular momentum" ($\mathbf{r} \times e\mathbf{A}$) must change by

$$-\frac{\hbar}{2}$$

$$\Delta L = \frac{\hbar}{2} - \mathbf{r} \times e\mathbf{A} \quad (32)$$

$$= \left[\frac{\hbar}{2} - \frac{e\phi}{2\pi} \right] \hat{z} \quad (33)$$

In order that the change of angular momentum, ΔL , equals zero, ϕ must be

- 5 $\Phi_0 = \frac{h}{2e}$, the magnetic flux quantum. The magnetic moment of the electron is parallel or antiparallel to the applied field only. During the spin-flip transition, power must be conserved. Power flow is governed by the Poynting power theorem,

$$\nabla \cdot (\mathbf{E} \times \mathbf{H}) = -\frac{\partial}{\partial t} \left[\frac{1}{2} \mu_0 \mathbf{H} \cdot \mathbf{H} \right] - \frac{\partial}{\partial t} \left[\frac{1}{2} \epsilon_0 \mathbf{E} \cdot \mathbf{E} \right] - \mathbf{J} \cdot \mathbf{E} \quad (34)$$

- Eq. (35) gives the total energy of the flip transition which is the sum of the energy of
10 reorientation of the magnetic moment (1st term), the magnetic energy (2nd term), the electric energy (3rd term), and the dissipated energy of a fluxon treading the orbitsphere (4th term), respectively,

$$\Delta E_{mag}^{spin} = 2 \left(1 + \frac{\alpha}{2\pi} + \frac{2}{3} \alpha^2 \left(\frac{\alpha}{2\pi} \right) - \frac{4}{3} \left(\frac{\alpha}{2\pi} \right)^2 \right) \mu_B B \quad (35)$$

15 $\Delta E_{mag}^{spin} = g \mu_B B \quad (36)$

where the stored magnetic energy corresponding to the $\frac{\partial}{\partial t} \left[\frac{1}{2} \mu_0 \mathbf{H} \cdot \mathbf{H} \right]$ term

increases, the stored electric energy corresponding to the $\frac{\partial}{\partial t} \left[\frac{1}{2} \epsilon_0 \mathbf{E} \cdot \mathbf{E} \right]$ term

increases, and the $\mathbf{J} \cdot \mathbf{E}$ term is dissipative. The spin-flip transition can be considered as involving a magnetic moment of g times that of a Bohr magneton.

- 20 The g factor is redesignated the fluxon g factor as opposed to the anomalous g factor. Using $\alpha^{-1} = 137.03603(82)$, the calculated value of $\frac{g}{2}$ is 1.001 159 652 137.

The experimental value [23] of $\frac{g}{2}$ is 1.001 159 652 188(4).

SPIN AND ORBITAL PARAMETERS

25

The total function that describes the spinning motion of each electron orbitsphere is composed of two functions. One function, the spin function, is spatially uniform over the orbitsphere, spins with a quantized angular velocity, and gives rise to spin angular momentum. The other function, the modulation function,
30 can be spatially uniform—in which case there is no orbital angular momentum and the magnetic moment of the electron orbitsphere is one Bohr magneton—or not spatially uniform—in which case there is orbital angular momentum. The modulation

function also rotates with a quantized angular velocity.

The spin function of the electron corresponds to the nonradiative $n = 1$, $\ell = 0$ state of atomic hydrogen which is well known as an s state or orbital. (See Figure 1 for the charge function and Figure 2 for the current function.) In cases of orbitals of heavier elements and excited states of one electron atoms and atoms or ions of heavier elements with the ℓ quantum number not equal to zero and which are not constant as given by Eq. (13), the constant spin function is modulated by a time and spherical harmonic function as given by Eq. (14) and shown in Figure 3. The modulation or traveling charge density wave corresponds to an orbital angular momentum in addition to a spin angular momentum. These states are typically referred to as p, d, f, etc. orbitals. Application of Haus's [16] condition also predicts nonradiation for a constant spin function modulated by a time and spherically harmonic orbital function. There is acceleration without radiation as also shown in the Nonradiation Based on the Electron Electromagnetic Fields and the Poynting Power Vector section. (Also see Pearle, Abbott and Griffiths, Goedecke, and Daboul and Jensen [14, 19-21]). However, in the case that such a state arises as an excited state by photon absorption, it is radiative due to a radial dipole term in its current density function since it possesses spacetime Fourier Transform components synchronous with waves traveling at the speed of light [16]. (See Instability of Excited States section of Ref. [4].)

Moment of Inertia and Spin and Rotational Energies

The moments of inertia and the rotational energies as a function of the ℓ quantum number for the solutions of the time-dependent electron charge density functions (Eqs. (13-14)) given in the Angular Functions section are solved using the rigid rotor equation [24]. The details of the derivations of the results as well as the demonstration that Eqs. (13-14) with the results given *infra.* are solutions of the wave equation are given in Chp 1, Rotational Parameters of the Electron (Angular Momentum, Rotational Energy, Moment of Inertia) section, of Ref. [4].

$$\ell = 0$$

$$I_z = I_{spin} = \frac{m_e r_n^2}{2} \quad (37)$$

$$L_z = I\omega_z = \pm \frac{\hbar}{2} \quad (38)$$

$$E_{\text{rotational}} = E_{\text{rotational, spin}} = \frac{1}{2} \left[I_{\text{spin}} \left(\frac{\hbar}{m_e r_n^2} \right)^2 \right] = \frac{1}{2} \left[\frac{m_e r_n^2}{2} \left(\frac{\hbar}{m_e r_n^2} \right)^2 \right] = \frac{1}{4} \left[\frac{\hbar^2}{2 I_{\text{spin}}} \right] \quad (39)$$

1 ? 0

$$5 \quad I_{\text{orbital}} = m_e r_n^2 \left[\frac{\ell(\ell+1)}{\ell^2 + \ell + 1} \right]^{\frac{1}{2}} \quad (40)$$

$$L_z = m \hbar \quad (41)$$

$$L_{z \text{ total}} = L_{z \text{ spin}} + L_{z \text{ orbital}} \quad (42)$$

$$E_{\text{rotational, orbital}} = \frac{\hbar^2}{2I} \left[\frac{\ell(\ell+1)}{\ell^2 + 2\ell + 1} \right] \quad (43)$$

$$T = \frac{\hbar^2}{2m_e r_n^2} \quad (44)$$

$$10 \quad \langle E_{\text{rotational, orbital}} \rangle = 0 \quad (45)$$

From Eq. (45), the time average rotational energy is zero; thus, the principal levels are degenerate except when a magnetic field is applied.

15 FORCE BALANCE EQUATION

The radius of the nonradiative ($n = 1$) state is solved using the electromagnetic force equations of Maxwell relating the charge and mass density functions wherein the angular momentum of the electron is given by Planck's constant bar [4]. The reduced mass arises naturally from an electrodynamic interaction between the electron and the proton of mass m_p .

$$\frac{m_e}{4\pi r_1^2} \frac{v_1^2}{r_1} = \frac{e}{4\pi r_1^2} \frac{Ze}{4\pi \epsilon_0 r_1^2} - \frac{1}{4\pi r_1^2} \frac{\hbar^2}{m_p r_n^3} \quad (46)$$

$$r_1 = \frac{a_H}{Z} \quad (47)$$

where a_H is the radius of the hydrogen atom.

25 ENERGY CALCULATIONS

From Maxwell's equations, the potential energy V , kinetic energy T , electric energy or binding energy E_{ele} are

$$V = \frac{-Ze^2}{4\pi \epsilon_0 r_1} = \frac{-Z^2 e^2}{4\pi \epsilon_0 a_H} = -Z^2 \times 4.3675 \times 10^{-18} \text{ J} = -Z^2 \times 27.2 \text{ eV} \quad (48)$$

$$30 \quad T = \frac{Z^2 e^2}{8\pi \epsilon_0 a_H} = Z^2 \times 13.59 \text{ eV} \quad (49)$$

$$T = E_{\text{ele}} = -\frac{1}{2} \epsilon_0 \int_{\infty}^{r_1} E^2 dv \quad \text{where } E = -\frac{Ze}{4\pi \epsilon_0 r^2} \quad (50)$$

$$E_{cle} = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_H} = -Z^2 \times 2.1786 \times 10^{-18} \text{ J} = -Z^2 \times 13.598 \text{ eV} \quad (51)$$

The calculated Rydberg constant is $10,967,758 \text{ m}^{-1}$; the experimental Rydberg constant is $10,967,758 \text{ m}^{-1}$. For increasing Z , the velocity becomes a significant fraction of the speed of light; thus, special relativistic corrections were included in the calculation of the ionization energies of one-electron atoms that are given in TABLE I.

TABLE I. Relativistically corrected ionization energies for some one-electron atoms.

| One e Atom | Z | γ^* ^a | Theoretical Ionization Energies (eV) ^b | Experimental Ionization Energies (eV) ^c | Relative Difference between Experimental and Calculated ^d |
|-------------------|----|-------------------------|--|---|--|
| H | 1 | 1.000007 | 13.59838 | 13.59844 | 0.00000 |
| He ⁺ | 2 | 1.000027 | 54.40941 | 54.41778 | 0.00015 |
| Li ²⁺ | 3 | 1.000061 | 122.43642 | 122.45429 | 0.00015 |
| Be ³⁺ | 4 | 1.000109 | 217.68510 | 217.71865 | 0.00015 |
| B ⁴⁺ | 5 | 1.000172 | 340.16367 | 340.2258 | 0.00018 |
| C ⁵⁺ | 6 | 1.000251 | 489.88324 | 489.99334 | 0.00022 |
| N ⁶⁺ | 7 | 1.000347 | 666.85813 | 667.046 | 0.00028 |
| O ⁷⁺ | 8 | 1.000461 | 871.10635 | 871.4101 | 0.00035 |
| F ⁸⁺ | 9 | 1.000595 | 1102.65013 | 1103.1176 | 0.00042 |
| Ne ⁹⁺ | 10 | 1.000751 | 1361.51654 | 1362.1995 | 0.00050 |
| Na ¹⁰⁺ | 11 | 1.000930 | 1647.73821 | 1648.702 | 0.00058 |
| Mg ¹¹⁺ | 12 | 1.001135 | 1961.35405 | 1962.665 | 0.00067 |
| Al ¹²⁺ | 13 | 1.001368 | 2302.41017 | 2304.141 | 0.00075 |
| Si ¹³⁺ | 14 | 1.001631 | 2670.96078 | 2673.182 | 0.00083 |
| P ¹⁴⁺ | 15 | 1.001927 | 3067.06918 | 3069.842 | 0.00090 |
| S ¹⁵⁺ | 16 | 1.002260 | 3490.80890 | 3494.1892 | 0.00097 |
| Cl ¹⁶⁺ | 17 | 1.002631 | 3942.26481 | 3946.296 | 0.00102 |
| Ar ¹⁷⁺ | 18 | 1.003045 | 4421.53438 | 4426.2296 | 0.00106 |
| K ¹⁸⁺ | 19 | 1.003505 | 4928.72898 | 4934.046 | 0.00108 |
| Ca ¹⁹⁺ | 20 | 1.004014 | 5463.97524 | 5469.864 | 0.00108 |
| Sc ²⁰⁺ | 21 | 1.004577 | 6027.41657 | 6033.712 | 0.00104 |
| Ti ²¹⁺ | 22 | 1.005197 | 6619.21462 | 6625.82 | 0.00100 |
| V ²²⁺ | 23 | 1.005879 | 7239.55091 | 7246.12 | 0.00091 |
| Cr ²³⁺ | 24 | 1.006626 | 7888.62855 | 7894.81 | 0.00078 |
| Mn ²⁴⁺ | 25 | 1.007444 | 8566.67392 | 8571.94 | 0.00061 |
| Fe ²⁵⁺ | 26 | 1.008338 | 9273.93857 | 9277.69 | 0.00040 |
| Co ²⁶⁺ | 27 | 1.009311 | 10010.70111 | 10012.12 | 0.00014 |
| Ni ²⁷⁺ | 28 | 1.010370 | 10777.26918 | 10775.4 | -0.00017 |
| Cu ²⁸⁺ | 29 | 1.011520 | 11573.98161 | 11567.617 | -0.00055 |

^a Eq. (1.250) (follows Eqs. (5), (15), and (47)).^b Eq. (1.251) (Eq. (51) times γ^*).5 ^c From theoretical calculations, interpolation of H isoelectronic and Rydberg series, and experimental data [24-25].^d (Experimental-theoretical)/experimental.

TWO ELECTRON ATOMS

- Two electron atoms may be solved from a central force balance equation with
 5 the nonradiation condition [4]. The force balance equation is

$$\frac{m_e v_2^2}{4\pi r_2^2} = \frac{e}{4\pi r_2^2} \frac{(Z-1)e}{4\pi\epsilon_0 r_2^2} + \frac{1}{4\pi r_2^2} \frac{\hbar^2}{Zm_e r_2^3} \sqrt{s(s+1)} \quad (52)$$

which gives the radius of both electrons as

$$r_2 = r_1 = a_0 \left(\frac{1}{Z-1} - \frac{\sqrt{s(s+1)}}{Z(Z-1)} \right); s = \frac{1}{2} \quad (53)$$

10 IONIZATION ENERGIES CALCULATED USING THE POYNTING POWER THEOREM

For helium, which has no electric field beyond r_1

$$Ionization\ Energy(He) = -E(electric) + E(magnetic) \quad (54)$$

- 15 where,

$$E(electric) = -\frac{(Z-1)e^2}{8\pi\epsilon_0 r_1} \quad (55)$$

$$E(magnetic) = \frac{2\pi\mu_0 e^2 \hbar^2}{m_e^2 r_1^3} \quad (56)$$

For $3 \leq Z$

$$Ionization\ Energy = -Electric\ Energy - \frac{1}{Z} Magnetic\ Energy \quad (57)$$

- 20 For increasing Z , the velocity becomes a significant fraction of the speed of light; thus, special relativistic corrections were included in the calculation of the ionization energies of two-electron atoms that are given in TABLE II.

TABLE II. Relativistically corrected ionization energies for some two-electron atoms.

| 2 e Atom | Z | r_1 (a_0) ^a | Electric Energy ^b (eV) | Magnetic Energy ^c (eV) |
|--------------------------|----|---------------------------------|---|---|
| <i>He</i> | 2 | 0.566987 | 23.996467 | 0.590536 |
| <i>Li</i> ⁺ | 3 | 0.35566 | 76.509 | 2.543 |
| <i>Be</i> ²⁺ | 4 | 0.26116 | 156.289 | 6.423 |
| <i>B</i> ³⁺ | 5 | 0.20670 | 263.295 | 12.956 |
| <i>C</i> ⁴⁺ | 6 | 0.17113 | 397.519 | 22.828 |
| <i>N</i> ⁵⁺ | 7 | 0.14605 | 558.958 | 36.728 |
| <i>O</i> ⁶⁺ | 8 | 0.12739 | 747.610 | 55.340 |
| <i>F</i> ⁷⁺ | 9 | 0.11297 | 963.475 | 79.352 |
| <i>Ne</i> ⁸⁺ | 10 | 0.10149 | 1206.551 | 109.451 |
| <i>Na</i> ⁹⁺ | 11 | 0.09213 | 1476.840 | 146.322 |
| <i>Mg</i> ¹⁰⁺ | 12 | 0.08435 | 1774.341 | 190.652 |
| <i>Al</i> ¹¹⁺ | 13 | 0.07778 | 2099.05 | 243.13 |
| <i>Si</i> ¹²⁺ | 14 | 0.07216 | 2450.98 | 304.44 |
| <i>P</i> ¹³⁺ | 15 | 0.06730 | 2830.11 | 375.26 |
| <i>S</i> ¹⁴⁺ | 16 | 0.06306 | 3236.46 | 456.30 |
| <i>Cl</i> ¹⁵⁺ | 17 | 0.05932 | 3670.02 | 548.22 |
| <i>Ar</i> ¹⁶⁺ | 18 | 0.05599 | 4130.79 | 651.72 |
| <i>K</i> ¹⁷⁺ | 19 | 0.05302 | 4618.77 | 767.49 |
| <i>Ca</i> ¹⁸⁺ | 20 | 0.05035 | 5133.96 | 896.20 |
| <i>Sc</i> ¹⁹⁺ | 21 | 0.04794 | 5676.37 | 1038.56 |
| <i>Ti</i> ²⁰⁺ | 22 | 0.04574 | 6245.98 | 1195.24 |
| <i>V</i> ²¹⁺ | 23 | 0.04374 | 6842.81 | 1366.92 |
| <i>Cr</i> ²²⁺ | 24 | 0.04191 | 7466.85 | 1554.31 |
| <i>Mn</i> ²³⁺ | 25 | 0.04022 | 8118.10 | 1758.08 |
| <i>Fe</i> ²⁴⁺ | 26 | 0.03867 | 8796.56 | 1978.92 |
| <i>Co</i> ²⁵⁺ | 27 | 0.03723 | 9502.23 | 2217.51 |
| <i>Ni</i> ²⁶⁺ | 28 | 0.03589 | 10235.12 | 2474.55 |
| <i>Cu</i> ²⁷⁺ | 29 | 0.03465 | 10995.21 | 2750.72 |

| 2 e Atom | Z | Velocity (m/s) d | γ^* e | Theoretical Ionization Energies f (eV) | Experimental Ionization Energies g (eV) | Relative Error h |
|-------------------|----|---------------------|--------------|---|--|---------------------|
| He | 2 | 3.85845E+06 | 1.00002 | 24.58750 | 24.58741 | -0.000004 |
| Li ⁺ | 3 | 6.15103E+06 | 1.00005 | 75.665 | 75.64018 | -0.0003 |
| Be ²⁺ | 4 | 8.37668E+06 | 1.00010 | 154.699 | 153.89661 | -0.0052 |
| B ³⁺ | 5 | 1.05840E+07 | 1.00016 | 260.746 | 259.37521 | -0.0053 |
| C ⁴⁺ | 6 | 1.27836E+07 | 1.00024 | 393.809 | 392.087 | -0.0044 |
| N ⁵⁺ | 7 | 1.49794E+07 | 1.00033 | 553.896 | 552.0718 | -0.0033 |
| O ⁶⁺ | 8 | 1.71729E+07 | 1.00044 | 741.023 | 739.29 | -0.0023 |
| F ⁷⁺ | 9 | 1.93649E+07 | 1.00057 | 955.211 | 953.9112 | -0.0014 |
| Ne ⁸⁺ | 10 | 2.15560E+07 | 1.00073 | 1196.483 | 1195.8286 | -0.0005 |
| Na ⁹⁺ | 11 | 2.37465E+07 | 1.00090 | 1464.871 | 1465.121 | 0.0002 |
| Mg ¹⁰⁺ | 12 | 2.59364E+07 | 1.00110 | 1760.411 | 1761.805 | 0.0008 |
| Al ¹¹⁺ | 13 | 2.81260E+07 | 1.00133 | 2083.15 | 2085.98 | 0.0014 |
| Si ¹²⁺ | 14 | 3.03153E+07 | 1.00159 | 2433.13 | 2437.63 | 0.0018 |
| P ¹³⁺ | 15 | 3.25043E+07 | 1.00188 | 2810.42 | 2816.91 | 0.0023 |
| S ¹⁴⁺ | 16 | 3.46932E+07 | 1.00221 | 3215.09 | 3223.78 | 0.0027 |
| Cl ¹⁵⁺ | 17 | 3.68819E+07 | 1.00258 | 3647.22 | 3658.521 | 0.0031 |
| Ar ¹⁶⁺ | 18 | 3.90705E+07 | 1.00298 | 4106.91 | 4120.8857 | 0.0034 |
| K ¹⁷⁺ | 19 | 4.12590E+07 | 1.00344 | 4594.25 | 4610.8 | 0.0036 |
| Ca ¹⁸⁺ | 20 | 4.34475E+07 | 1.00394 | 5109.38 | 5128.8 | 0.0038 |
| Sc ¹⁹⁺ | 21 | 4.56358E+07 | 1.00450 | 5652.43 | 5674.8 | 0.0039 |
| Ti ²⁰⁺ | 22 | 4.78241E+07 | 1.00511 | 6223.55 | 6249 | 0.0041 |
| V ²¹⁺ | 23 | 5.00123E+07 | 1.00578 | 6822.93 | 6851.3 | 0.0041 |
| Cr ²²⁺ | 24 | 5.22005E+07 | 1.00652 | 7450.76 | 7481.7 | 0.0041 |
| Mn ²³⁺ | 25 | 5.43887E+07 | 1.00733 | 8107.25 | 8140.6 | 0.0041 |
| Fe ²⁴⁺ | 26 | 5.65768E+07 | 1.00821 | 8792.66 | 8828 | 0.0040 |
| Co ²⁵⁺ | 27 | 5.87649E+07 | 1.00917 | 9507.25 | 9544.1 | 0.0039 |
| Ni ²⁶⁺ | 28 | 6.09529E+07 | 1.01022 | 10251.33 | 10288.8 | 0.0036 |
| Cu ²⁷⁺ | 29 | 6.31409E+07 | 1.01136 | 11025.21 | 11062.38 | 0.0034 |

a From Eq. (7.19) (Eq. (53)).

b From Eq. (7.29) (Eq. (61)).

c From Eq. (7.30).

5 d From Eq. (7.31).

e From Eq. (1.250) with the velocity given by Eq. (7.31).

f From Eqs. (7.28) and (7.47) with $E(\text{electric})$ of Eq. (7.29) relativistically corrected by γ^* according to Eq. (1.251) except that the electron-nuclear electrodynamic relativistic factor corresponding to the reduced mass of Eqs. (1.213-1.223) was not included.

10 g From theoretical calculations for ions Ne^{8+} to Cu^{28+} [24-25].

h (Experimental-theoretical)/experimental.

APPROACH FOR THREE-THROUGH TWENTY-ELECTRON ATOMS

For each two-electron atom having a central charge of Z times that of the proton, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by Eq. (53). For $Z \geq 3$, the next electron which binds to form the corresponding three-electron atom is attracted by the central Coulomb field and is repelled by diamagnetic forces due to the spin-paired inner electrons such that it forms an unpaired orbitsphere at radius r_3 . Since the charge-density function of each s electron including those of three-electron atoms is spherically symmetrical, the central Coulomb force, F_{ele} , that acts on the outer electron to cause it to bind due to the nucleus and the inner electrons is given by

$$F_{ele} = \frac{(Z-n)e^2}{4\pi\epsilon_0 r_n^2} \hat{i}_r \quad (58)$$

for $r > r_{n-1}$ where n corresponds to the number of electrons of the atom and Z is its atomic number. In each case, the magnetic field of the binding outer electron changes the angular velocities of the inner electrons. However, in each case, the magnetic field of the outer electron provides a central Lorentzian force which exactly balances the change in centrifugal force because of the change in angular velocity [4]. The inner electrons remain at their initial radii, but cause a diamagnetic force according to Lenz's law or a paramagnetic force depending on the spin and orbital angular momenta of the inner electrons and that of the outer. The force balance minimizes the energy of the atom.

It was shown previously [4] that the same principles including the central force given by Eq. (58) applies in the case that a nonuniform distribution of charge according to Eq. (14) achieves an energy minimum. In the case that an electron has orbital angular momentum in addition to spin angular momentum, the corresponding charge density wave is a time and spherical-harmonic wherein the traveling charge-density wave modulates the constant charge-density function as given in the Angular Functions section. It was found that electrostatic and magnetostatic s electrons pair in shells until a fifth electron is added. Then, a nonuniform distribution of charge achieves an energy minimum with the formation of a third shell due to the dependence of the magnetic forces on the nuclear charge and orbital energy (Eqs. (10.52), (10.55), and (10.93) of Ref. [4]). Minimum energy configurations are given by solutions to Laplace's equation. The general form of the solution is

$$\Phi(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} B_{\ell, m} r^{-(\ell+1)} Y_{\ell}^m(\theta, \phi) \quad (59)$$

As demonstrated previously, this general solution also gives the functions of the resonant photons of excited states [4]. To maintain the symmetry of the central charge and the energy minimum condition given by solutions to Laplace's equation (Eq. (59)), the charge-density waves on electron orbitspheres at r_1 and r_3 complement those of the outer orbitals when the outer p orbitals are not all occupied by at least one electron, and the complementary charge-density waves are provided by electrons at r_3 when this condition is met. Since the angular harmonic charge-density waves are nonradiative as shown in the Nonradiation Based on the Electron Electromagnetic Fields and the Poynting Power Vector section, the time-averaged central field is inverse r -squared even though the central field is modulated by the concentric charge-density waves. The modulated central field maintains the spherical harmonic orbitals that maintain the spherical-harmonic phase according to Eq. (59). Thus, the central Coulomb force, F_{ele} , that acts on the outer electron to cause it to bind due to the nucleus and the inner electrons is given by Eq. (58).

The outer electrons of atoms and ions that are isoelectronic with the series boron through neon half-fill a 2p level with unpaired electrons at nitrogen, then fill the level with paired electrons at neon. In general, electrons of an atom with the same principal and l quantum numbers align parallel until each of the m_l levels are occupied, and then pairing occurs until each of the m_l levels contain paired electrons. The electron configuration for one through twenty-electron atoms that achieves an energy minimum is: $1s < 2s < 2p < 3s < 3p < 4s$. In each case, the force balance of the central Coulombic, paramagnetic, and diamagnetic forces was derived for each n-electron atom that was solved for the radius of each electron. The ionization energies were obtained using the calculated radii in the determination of the Coulombic and any magnetic energies. The radii and ionization energies for all cases were given by equations having fundamental constants and each nuclear charge, Z , only. The predicted ionization energies and electron configurations compared with the experimental values [24-26] are given in TABLE I-XXIII.

The predicted electron configurations are in agreement with the experimental configurations known for 400 atoms and ions. The agreement between the experimental and calculated values of the ionization energies given in TABLE I-XX is well within the experimental capability of the spectroscopic determinations

- including the values at large Z which relies on X-ray spectroscopy. Ionization energies are difficult to determine since the cut-off of the Rydberg series of lines at the ionization energy is often not observed. Thus, each series isoelectronic with the neutral n -electron atom given in TABLES I-XX [24-25] relies on theoretical
- 5 calculations and interpolation of the isoelectronic and Rydberg series as well as direct experimental data to extend the precision beyond the capability of X-ray spectroscopy. But, no assurances can be given that these techniques are correct, and they may not improve the results. In each case, the error given in the last column of TABLES I-XX is very reasonable given the quality of the data.

TABLE III. Ionization energies for some three-electron atoms.

| 3 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | Electric Energy c (eV) | Δv d (m/s) | ΔE_T e (eV) | Theoretic al Ionization Energies f (eV) | Experime ntal Ionization Energies g (eV) | Relative Error h |
|-------------------|----|----------------------|----------------------|------------------------------|-----------------------|------------------------|---|---|---------------------|
| Li | 3 | 0.35566 | 2.55606 | 5.3230 | 1.657 1E+04 | 1.5613E -03 | 5.40381 | 5.39172 | -0.00224 |
| Be ⁺ | 4 | 0.26116 | 1.49849 | 18.1594 | 4.434 6E+04 | 1.1181E -02 | 18.1706 | 18.21116 | 0.00223 |
| B ²⁺ | 5 | 0.20670 | 1.07873 | 37.8383 | 7.446 0E+04 | 3.1523E -02 | 37.8701 | 37.93064 | 0.00160 |
| C ³⁺ | 6 | 0.17113 | 0.84603 | 64.3278 | 1.058 0E+05 | 6.3646E -02 | 64.3921 | 64.4939 | 0.00158 |
| N ⁴⁺ | 7 | 0.14605 | 0.69697 | 97.6067 | 1.378 2E+05 | 1.0800E -01 | 97.7160 | 97.8902 | 0.00178 |
| O ⁵⁺ | 8 | 0.12739 | 0.59299 | 137.6655 | 1.702 6E+05 | 1.6483E -01 | 137.8330 | 138.1197 | 0.00208 |
| F ⁶⁺ | 9 | 0.11297 | 0.51621 | 184.5001 | 2.029 8E+05 | 2.3425E -01 | 184.7390 | 185.186 | 0.00241 |
| Ne ⁷⁺ | 10 | 0.10149 | 0.45713 | 238.1085 | 2.358 9E+05 | 3.1636E -01 | 238.4325 | 239.0989 | 0.00279 |
| Na ⁸⁺ | 11 | 0.09213 | 0.41024 | 298.4906 | 2.689 4E+05 | 4.1123E -01 | 298.9137 | 299.864 | 0.00317 |
| Mg ⁹⁺ | 12 | 0.08435 | 0.37210 | 365.6469 | 3.021 0E+05 | 5.1890E -01 | 366.1836 | 367.5 | 0.00358 |
| Al ¹⁰⁺ | 13 | 0.07778 | 0.34047 | 439.5790 | 3.353 5E+05 | 6.3942E -01 | 440.2439 | 442 | 0.00397 |
| Si ¹¹⁺ | 14 | 0.07216 | 0.31381 | 520.2888 | 3.686 8E+05 | 7.7284E -01 | 521.0973 | 523.42 | 0.00444 |
| P ¹²⁺ | 15 | 0.06730 | 0.29102 | 607.7792 | 4.020 8E+05 | 9.1919E -01 | 608.7469 | 611.74 | 0.00489 |
| S ¹³⁺ | 16 | 0.06306 | 0.27132 | 702.0535 | 4.355 4E+05 | 1.0785E +00 | 703.1966 | 707.01 | 0.00539 |
| Cl ¹⁴⁺ | 17 | 0.05932 | 0.25412 | 803.1158 | 4.690 5E+05 | 1.2509E +00 | 804.4511 | 809.4 | 0.00611 |
| Ar ¹⁵⁺ | 18 | 0.05599 | 0.23897 | 910.9708 | 5.026 2E+05 | 1.4364E +00 | 912.5157 | 918.03 | 0.00601 |
| K ¹⁶⁺ | 19 | 0.05302 | 0.22552 | 1025.624 | 5.362 5E+05 | 1.6350E +00 | 1027.396 | 1033.4 | 0.00581 |
| Ca ¹⁷⁺ | 20 | 0.05035 | 0.21350 | 1147.081 | 5.699 9 3E+05 | 1.8468E +00 | 1149.101 | 1157.8 | 0.00751 |
| Sc ¹⁸⁺ | 21 | 0.04794 | 0.20270 | 1275.351 | 6.036 6 7E+05 | 2.0720E +00 | 1277.636 | 1287.97 | 0.00802 |
| Ti ¹⁹⁺ | 22 | 0.04574 | 0.19293 | 1410.441 | 6.374 4 8E+05 | 2.3106E +00 | 1413.012 | 1425.4 | 0.00869 |
| V ²⁰⁺ | 23 | 0.04374 | 0.18406 | 1552.360 | 6.713 6 5E+05 | 2.5626E +00 | 1555.239 | 1569.6 | 0.00915 |
| Cr ²¹⁺ | 24 | 0.04191 | 0.17596 | 1701.119 | 7.053 7 0E+05 | 2.8283E +00 | 1704.328 | 1721.4 | 0.00992 |
| Mn ²²⁺ | 25 | 0.04022 | 0.16854 | 1856.730 | 7.393 1 2E+05 | 3.1077E +00 | 1860.292 | 1879.9 | 0.01043 |
| Fe ²³⁺ | 26 | 0.03867 | 0.16172 | 2019.205 | 7.734 | 3.4011E | 2023.145 | 2023 | -0.00007 |

| | | | | | | | | | |
|------------|----|---------|---------|----------|-------|---------|----------|--------|---------|
| | | | | 0 | 2E+05 | +00 | 1 | | |
| Co^{24+} | 27 | 0.03723 | 0.15542 | 2188.558 | 8.076 | 3.7084E | 2192.902 | 2219 | 0.01176 |
| | | | | 5 | 2E+05 | +00 | 0 | | |
| Ni^{25+} | 28 | 0.03589 | 0.14959 | 2364.806 | 8.419 | 4.0300E | 2369.580 | 2399.2 | 0.01235 |
| | | | | 5 | 1E+05 | +00 | 3 | | |
| Cu^{26+} | 29 | 0.03465 | 0.14418 | 2547.966 | 8.763 | 4.3661E | 2553.198 | 2587.5 | 0.01326 |
| | | | | 4 | 0E+05 | +00 | 7 | | |

^a Radius of the paired inner electrons of three-electron atoms from Eq. (10.49) (Eq. (60)).

^b Radius of the unpaired outer electron of three-electron atoms from Eq. (10.50) (Eq. (60)).

5 ^c Electric energy of the outer electron of three-electron atoms from Eq. (10.43) (Eq. (61)).

^d Change in the velocity of the paired inner electrons due to the unpaired outer electron of three-electron atoms from Eq. (10.46).

10 ^e Change in the kinetic energy of the paired inner electrons due to the unpaired outer electron of three-electron atoms from Eq. (10.47).

^f Calculated ionization energies of three-electron atoms from Eq. (10.48) for $Z > 3$ and Eq. (10.25) for Li .

^g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

15 ^h (Experimental-theoretical)/experimental.

TABLE IV. Ionization energies for some four-electron atoms.

| 4 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | Electric Energy c (eV) | Magneti c Energy d (eV) | Δv e (m/s X 10^{-3}) | ΔE_T f (eV) | Theoretic al Ionizatio n Energies g (eV) | Experim ental Ionizatio n Energies h (eV) | Relative Error i |
|-------------------------|----|----------------------|----------------------|---------------------------------|-------------------------------------|---------------------------------------|------------------------|--|---|---------------------|
| <i>Be</i> | 4 | 0.2611 6 | 1.5250 3 | 8.9178 | 0.03226 | 0.4207 | 0.0101 | 9.28430 | 9.32263 | 0.0041 |
| <i>B⁺</i> | 5 | 0.2067 0 | 1.0793 0 | 25.2016 | 0.0910 | 0.7434 | 0.0314 | 25.1627 | 25.1548 4 | -0.0003 |
| <i>C²⁺</i> | 6 | 0.1711 3 | 0.8431 7 | 48.3886 | 0.1909 | 1.0688 | 0.0650 | 48.3125 | 47.8878 | -0.0089 |
| <i>N³⁺</i> | 7 | 0.1460 5 | 0.6938 5 | 78.4029 | 0.3425 | 1.3969 | 0.1109 | 78.2765 | 77.4735 | -0.0104 |
| <i>O⁴⁺</i> | 8 | 0.1273 9 | 0.5902 0 | 115.214 8 | 0.5565 | 1.7269 | 0.1696 | 115.024 9 | 113.899 | -0.0099 |
| <i>F⁵⁺</i> | 9 | 0.1129 7 | 0.5138 2 | 158.810 2 | 0.8434 | 2.0582 | 0.2409 | 158.543 4 | 157.165 1 | -0.0088 |
| <i>Ne⁶⁺</i> | 10 | 0.1014 9 | 0.4551 1 | 209.181 3 | 1.2138 | 2.3904 | 0.3249 | 208.824 3 | 207.275 9 | -0.0075 |
| <i>Na⁷⁺</i> | 11 | 0.0921 3 | 0.4085 3 | 266.323 3 | 1.6781 | 2.7233 | 0.4217 | 265.862 8 | 264.25 | -0.0061 |
| <i>Mg⁸⁺</i> | 12 | 0.0843 5 | 0.3706 5 | 330.233 5 | 2.2469 | 3.0567 | 0.5312 | 329.655 9 | 328.06 | -0.0049 |
| <i>Al⁹⁺</i> | 13 | 0.0777 8 | 0.3392 3 | 400.909 7 | 2.9309 | 3.3905 | 0.6536 | 400.201 7 | 398.75 | -0.0036 |
| <i>Si¹⁰⁺</i> | 14 | 0.0721 6 | 0.3127 4 | 478.350 7 | 3.7404 | 3.7246 | 0.7888 | 477.498 9 | 476.36 | -0.0024 |
| <i>P¹¹⁺</i> | 15 | 0.0673 0 | 0.2901 0 | 562.555 5 | 4.6861 | 4.0589 | 0.9367 | 561.546 4 | 560.8 | -0.0013 |
| <i>S¹²⁺</i> | 16 | 0.0630 6 | 0.2705 3 | 653.523 3 | 5.7784 | 4.3935 | 1.0975 | 652.343 6 | 652.2 | -0.0002 |
| <i>Cl¹³⁺</i> | 17 | 0.0593 2 | 0.2534 4 | 751.253 7 | 7.0280 | 4.7281 | 1.2710 | 749.889 9 | 749.76 | -0.0002 |
| <i>Ar¹⁴⁺</i> | 18 | 0.0559 9 | 0.2383 9 | 855.746 3 | 8.4454 | 5.0630 | 1.4574 | 854.184 9 | 854.77 | 0.0007 |
| <i>K¹⁵⁺</i> | 19 | 0.0530 2 | 0.2250 3 | 967.000 7 | 10.0410 | 5.3979 | 1.6566 | 965.228 3 | 968 | 0.0029 |
| <i>Ca¹⁶⁺</i> | 20 | 0.0503 5 | 0.2130 8 | 1085.01 67 | 11.8255 | 5.7329 | 1.8687 | 1083.01 98 | 1087 | 0.0037 |
| <i>Sc¹⁷⁺</i> | 21 | 0.0479 4 | 0.2023 5 | 1209.79 40 | 13.8094 | 6.0680 | 2.0935 | 1207.55 92 | 1213 | 0.0045 |
| <i>Ti¹⁸⁺</i> | 22 | 0.0457 4 | 0.1926 4 | 1341.33 26 | 16.0032 | 6.4032 | 2.3312 | 1338.84 65 | 1346 | 0.0053 |
| <i>V¹⁹⁺</i> | 23 | 0.0437 4 | 0.1838 3 | 1479.63 23 | 18.4174 | 6.7384 | 2.5817 | 1476.88 13 | 1486 | 0.0061 |
| <i>Cr²⁰⁺</i> | 24 | 0.0419 1 | 0.1757 9 | 1624.69 29 | 21.0627 | 7.0737 | 2.8450 | 1621.66 37 | 1634 | 0.0075 |
| <i>Mn²¹⁺</i> | 25 | 0.0402 2 | 0.1684 2 | 1776.51 44 | 23.9495 | 7.4091 | 3.1211 | 1773.19 35 | 1788 | 0.0083 |
| <i>Fe²²⁺</i> | 26 | 0.0386 7 | 0.1616 5 | 1935.09 68 | 27.0883 | 7.7444 | 3.4101 | 1931.47 07 | 1950 | 0.0095 |
| <i>Co²³⁺</i> | 27 | 0.0372 3 | 0.1554 0 | 2100.43 98 | 30.4898 | 8.0798 | 3.7118 | 2096.49 52 | 2119 | 0.0106 |

| | | | | | | | | | | |
|------------|----|--------|--------|---------|---------|--------|--------|---------|------|--------|
| Ni^{24+} | 28 | 0.0358 | 0.1496 | 2272.54 | 34.1644 | 8.4153 | 4.0264 | 2268.26 | 2295 | 0.0116 |
| | | 9 | 1 | 36 | | | | 69 | | |
| Cu^{25+} | 29 | 0.0346 | 0.1442 | 2451.40 | 38.1228 | 8.7508 | 4.3539 | 2446.78 | 2478 | 0.0126 |
| | | 5 | 4 | 80 | | | | 58 | | |

- a Radius of the paired inner electrons of four-electron atoms from Eq. (10.51) (Eq. (60)).
- b Radius of the paired outer electrons of four-electron atoms from Eq. (10.62) (Eq. (60)).
- 5 c Electric energy of the outer electrons of four-electron atoms from Eq. (10.63) (Eq. (61)).
- d Magnetic energy of the outer electrons of four-electron atoms upon unpairing from Eq. (7.30) and Eq. (10.64).
- 10 e Change in the velocity of the paired inner electrons due to the unpaired outer electron of four-electron atoms during ionization from Eq. (10.46).
- f Change in the kinetic energy of the paired inner electrons due to the unpaired outer electron of four-electron atoms during ionization from Eq. (10.47).
- g Calculated ionization energies of four-electron atoms from Eq. (10.68) for $Z > 4$ and Eq. (10.66) for Be .
- 15 h From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].
- i (Experimental-theoretical)/experimental.

TABLE V. Ionization energies for some five-electron atoms.

| 5 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_5 (a_0) ^c | Theoretical Ionization Energies ^d (eV) | Experimen tal Ionization Energies ^e (eV) | Relative Error ^f |
|-------------------|----|---------------------------------|---------------------------------|---------------------------------|--|---|--------------------------------|
| B | 5 | 0.20670 | 1.07930 | 1.67000 | 8.30266 | 8.29803 | -0.00056 |
| C ⁺ | 6 | 0.17113 | 0.84317 | 1.12092 | 24.2762 | 24.38332 | 0.0044 |
| N ²⁺ | 7 | 0.14605 | 0.69385 | 0.87858 | 46.4585 | 47.44924 | 0.0209 |
| O ³⁺ | 8 | 0.12739 | 0.59020 | 0.71784 | 75.8154 | 77.41353 | 0.0206 |
| F ⁴⁺ | 9 | 0.11297 | 0.51382 | 0.60636 | 112.1922 | 114.2428 | 0.0179 |
| Ne ⁵⁺ | 10 | 0.10149 | 0.45511 | 0.52486 | 155.5373 | 157.93 | 0.0152 |
| Na ⁶⁺ | 11 | 0.09213 | 0.40853 | 0.46272 | 205.8266 | 208.5 | 0.0128 |
| Mg ⁷⁺ | 12 | 0.08435 | 0.37065 | 0.41379 | 263.0469 | 265.96 | 0.0110 |
| Al ⁸⁺ | 13 | 0.07778 | 0.33923 | 0.37425 | 327.1901 | 330.13 | 0.0089 |
| Si ⁹⁺ | 14 | 0.07216 | 0.31274 | 0.34164 | 398.2509 | 401.37 | 0.0078 |
| P ¹⁰⁺ | 15 | 0.06730 | 0.29010 | 0.31427 | 476.2258 | 479.46 | 0.0067 |
| S ¹¹⁺ | 16 | 0.06306 | 0.27053 | 0.29097 | 561.1123 | 564.44 | 0.0059 |
| Cl ¹²⁺ | 17 | 0.05932 | 0.25344 | 0.27090 | 652.9086 | 656.71 | 0.0058 |
| Ar ¹³⁺ | 18 | 0.05599 | 0.23839 | 0.25343 | 751.6132 | 755.74 | 0.0055 |
| K ¹⁴⁺ | 19 | 0.05302 | 0.22503 | 0.23808 | 857.2251 | 861.1 | 0.0045 |
| Ca ¹⁵⁺ | 20 | 0.05035 | 0.21308 | 0.22448 | 969.7435 | 974 | 0.0044 |
| Sc ¹⁶⁺ | 21 | 0.04794 | 0.20235 | 0.21236 | 1089.1678 | 1094 | 0.0044 |
| Ti ¹⁷⁺ | 22 | 0.04574 | 0.19264 | 0.20148 | 1215.4975 | 1221 | 0.0045 |
| V ¹⁸⁺ | 23 | 0.04374 | 0.18383 | 0.19167 | 1348.7321 | 1355 | 0.0046 |
| Cr ¹⁹⁺ | 24 | 0.04191 | 0.17579 | 0.18277 | 1488.8713 | 1496 | 0.0048 |
| Mn ²⁰⁺ | 25 | 0.04022 | 0.16842 | 0.17466 | 1635.9148 | 1644 | 0.0049 |
| Fe ²¹⁺ | 26 | 0.03867 | 0.16165 | 0.16724 | 1789.8624 | 1799 | 0.0051 |
| Co ²²⁺ | 27 | 0.03723 | 0.15540 | 0.16042 | 1950.7139 | 1962 | 0.0058 |
| Ni ²³⁺ | 28 | 0.03589 | 0.14961 | 0.15414 | 2118.4690 | 2131 | 0.0059 |
| Cu ²⁴⁺ | 29 | 0.03465 | 0.14424 | 0.14833 | 2293.1278 | 2308 | 0.0064 |

^a Radius of the first set of paired inner electrons of five-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the second set of paired inner electrons of five-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the outer electron of five-electron atoms from Eq. (10.113) (Eq. (64)) for $Z > 5$ and Eq. (10.101) for B .

10 ^d Calculated ionization energies of five-electron atoms given by the electric energy (Eq. (10.114)) (Eq. (61)) for $Z > 5$ and Eq. (10.104) for B .

^e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^f (Experimental-theoretical)/experimental.

TABLE VI. Ionization energies for some six-electron atoms.

| 6 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | r_6 (a_0) c | Theoretical Ionization Energies d (eV) | Experimen tal Ionization Energies e (eV) | Relative Error f |
|-------------------|----|----------------------|----------------------|----------------------|---|--|---------------------|
| C | 6 | 0.17113 | 0.84317 | 1.20654 | 11.27671 | 11.2603 | -0.0015 |
| N ⁺ | 7 | 0.14605 | 0.69385 | 0.90119 | 30.1950 | 29.6013 | -0.0201 |
| O ²⁺ | 8 | 0.12739 | 0.59020 | 0.74776 | 54.5863 | 54.9355 | 0.0064 |
| F ³⁺ | 9 | 0.11297 | 0.51382 | 0.63032 | 86.3423 | 87.1398 | 0.0092 |
| Ne ⁴⁺ | 10 | 0.10149 | 0.45511 | 0.54337 | 125.1986 | 126.21 | 0.0080 |
| Na ⁵⁺ | 11 | 0.09213 | 0.40853 | 0.47720 | 171.0695 | 172.18 | 0.0064 |
| Mg ⁶⁺ | 12 | 0.08435 | 0.37065 | 0.42534 | 223.9147 | 225.02 | 0.0049 |
| Al ⁷⁺ | 13 | 0.07778 | 0.33923 | 0.38365 | 283.7121 | 284.66 | 0.0033 |
| Si ⁸⁺ | 14 | 0.07216 | 0.31274 | 0.34942 | 350.4480 | 351.12 | 0.0019 |
| P ⁹⁺ | 15 | 0.06730 | 0.29010 | 0.32081 | 424.1135 | 424.4 | 0.0007 |
| S ¹⁰⁺ | 16 | 0.06306 | 0.27053 | 0.29654 | 504.7024 | 504.8 | 0.0002 |
| Cl ¹¹⁺ | 17 | 0.05932 | 0.25344 | 0.27570 | 592.2103 | 591.99 | -0.0004 |
| Ar ¹²⁺ | 18 | 0.05599 | 0.23839 | 0.25760 | 686.6340 | 686.1 | -0.0008 |
| K ¹³⁺ | 19 | 0.05302 | 0.22503 | 0.24174 | 787.9710 | 786.6 | -0.0017 |
| Ca ¹⁴⁺ | 20 | 0.05035 | 0.21308 | 0.22772 | 896.2196 | 894.5 | -0.0019 |
| Sc ¹⁵⁺ | 21 | 0.04794 | 0.20235 | 0.21524 | 1011.3782 | 1009 | -0.0024 |
| Ti ¹⁶⁺ | 22 | 0.04574 | 0.19264 | 0.20407 | 1133.4456 | 1131 | -0.0022 |
| V ¹⁷⁺ | 23 | 0.04374 | 0.18383 | 0.19400 | 1262.4210 | 1260 | -0.0019 |
| Cr ¹⁸⁺ | 24 | 0.04191 | 0.17579 | 0.18487 | 1398.3036 | 1396 | -0.0017 |
| Mn ¹⁹⁺ | 25 | 0.04022 | 0.16842 | 0.17657 | 1541.0927 | 1539 | -0.0014 |
| Fe ²⁰⁺ | 26 | 0.03867 | 0.16165 | 0.16899 | 1690.7878 | 1689 | -0.0011 |
| Co ²¹⁺ | 27 | 0.03723 | 0.15540 | 0.16203 | 1847.3885 | 1846 | -0.0008 |
| Ni ²²⁺ | 28 | 0.03589 | 0.14961 | 0.15562 | 2010.8944 | 2011 | 0.0001 |
| Cu ²³⁺ | 29 | 0.03465 | 0.14424 | 0.14970 | 2181.3053 | 2182 | 0.0003 |

a Radius of the first set of paired inner electrons of six-electron atoms from Eq. (10.51) (Eq. (60)).

5 b Radius of the second set of paired inner electrons of six-electron atoms from Eq. (10.62) (Eq. (60)).

c Radius of the two unpaired outer electrons of six-electron atoms from Eq. (10.132) (Eq. (64)) for $Z > 6$ and Eq. (10.122) for C.

10 d Calculated ionization energies of six-electron atoms given by the electric energy (Eq. (10.133)) (Eq. (61)).

e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

f (Experimental-theoretical)/experimental.

TABLE VII. Ionization energies for some seven-electron atoms.

| 7 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_7 (a_0) ^c | Theoretical Ionization Energies ^d (eV) | Experimen tal Ionization Energies ^e (eV) | Relative Error ^f |
|-------------------|----|---------------------------------|---------------------------------|---------------------------------|--|---|--------------------------------|
| N | 7 | 0.14605 | 0.69385 | 0.93084 | 14.61664 | 14.53414 | -0.0057 |
| O ⁺ | 8 | 0.12739 | 0.59020 | 0.78489 | 34.6694 | 35.1173 | 0.0128 |
| F ²⁺ | 9 | 0.11297 | 0.51382 | 0.67084 | 60.8448 | 62.7084 | 0.0297 |
| Ne ³⁺ | 10 | 0.10149 | 0.45511 | 0.57574 | 94.5279 | 97.12 | 0.0267 |
| Na ⁴⁺ | 11 | 0.09213 | 0.40853 | 0.50250 | 135.3798 | 138.4 | 0.0218 |
| Mg ⁵⁺ | 12 | 0.08435 | 0.37065 | 0.44539 | 183.2888 | 186.76 | 0.0186 |
| Al ⁶⁺ | 13 | 0.07778 | 0.33923 | 0.39983 | 238.2017 | 241.76 | 0.0147 |
| Si ⁷⁺ | 14 | 0.07216 | 0.31274 | 0.36271 | 300.0883 | 303.54 | 0.0114 |
| P ⁸⁺ | 15 | 0.06730 | 0.29010 | 0.33191 | 368.9298 | 372.13 | 0.0086 |
| S ⁹⁺ | 16 | 0.06306 | 0.27053 | 0.30595 | 444.7137 | 447.5 | 0.0062 |
| Cl ¹⁰⁺ | 17 | 0.05932 | 0.25344 | 0.28376 | 527.4312 | 529.28 | 0.0035 |
| Ar ¹¹⁺ | 18 | 0.05599 | 0.23839 | 0.26459 | 617.0761 | 618.26 | 0.0019 |
| K ¹²⁺ | 19 | 0.05302 | 0.22503 | 0.24785 | 713.6436 | 714.6 | 0.0013 |
| Ca ¹³⁺ | 20 | 0.05035 | 0.21308 | 0.23311 | 817.1303 | 817.6 | 0.0006 |
| Sc ¹⁴⁺ | 21 | 0.04794 | 0.20235 | 0.22003 | 927.5333 | 927.5 | 0.0000 |
| Ti ¹⁵⁺ | 22 | 0.04574 | 0.19264 | 0.20835 | 1044.8504 | 1044 | -0.0008 |
| V ¹⁶⁺ | 23 | 0.04374 | 0.18383 | 0.19785 | 1169.0800 | 1168 | -0.0009 |
| Cr ¹⁷⁺ | 24 | 0.04191 | 0.17579 | 0.18836 | 1300.2206 | 1299 | -0.0009 |
| Mn ¹⁸⁺ | 25 | 0.04022 | 0.16842 | 0.17974 | 1438.2710 | 1437 | -0.0009 |
| Fe ¹⁹⁺ | 26 | 0.03867 | 0.16165 | 0.17187 | 1583.2303 | 1582 | -0.0008 |
| Co ²⁰⁺ | 27 | 0.03723 | 0.15540 | 0.16467 | 1735.0978 | 1735 | -0.0001 |
| Ni ²¹⁺ | 28 | 0.03589 | 0.14961 | 0.15805 | 1893.8726 | 1894 | 0.0001 |
| Cu ²²⁺ | 29 | 0.03465 | 0.14424 | 0.15194 | 2059.5543 | 2060 | 0.0002 |

^a Radius of the first set of paired inner electrons of seven-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the second set of paired inner electrons of seven-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three unpaired paired outer electrons of seven-electron atoms from Eq. (10.152) (Eq. (64)) for $Z > 7$ and Eq. (10.142) for N .

10 ^d Calculated ionization energies of seven-electron atoms given by the electric energy (Eq. (10.153)) (Eq. (61)).

^e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^f (Experimental-theoretical)/experimental.

TABLE VIII. Ionization energies for some eight-electron atoms.

| 8 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_8 (a_0) ^c | Theoretical Ionization Energies ^d (eV) | Experimen tal Ionization Energies ^e (eV) | Relative Error ^f |
|-------------------|----|---------------------------------|---------------------------------|---------------------------------|--|---|--------------------------------|
| O | 8 | 0.12739 | 0.59020 | 1.00000 | 13.60580 | 13.6181 | 0.0009 |
| F ⁺ | 9 | 0.11297 | 0.51382 | 0.7649 | 35.5773 | 34.9708 | -0.0173 |
| Ne ²⁺ | 10 | 0.10149 | 0.45511 | 0.6514 | 62.6611 | 63.45 | 0.0124 |
| Na ³⁺ | 11 | 0.09213 | 0.40853 | 0.5592 | 97.3147 | 98.91 | 0.0161 |
| Mg ⁴⁺ | 12 | 0.08435 | 0.37065 | 0.4887 | 139.1911 | 141.27 | 0.0147 |
| Al ⁵⁺ | 13 | 0.07778 | 0.33923 | 0.4338 | 188.1652 | 190.49 | 0.0122 |
| Si ⁶⁺ | 14 | 0.07216 | 0.31274 | 0.3901 | 244.1735 | 246.5 | 0.0094 |
| P ⁷⁺ | 15 | 0.06730 | 0.29010 | 0.3543 | 307.1791 | 309.6 | 0.0078 |
| S ⁸⁺ | 16 | 0.06306 | 0.27053 | 0.3247 | 377.1579 | 379.55 | 0.0063 |
| Cl ⁹⁺ | 17 | 0.05932 | 0.25344 | 0.2996 | 454.0940 | 455.63 | 0.0034 |
| Ar ¹⁰⁺ | 18 | 0.05599 | 0.23839 | 0.2782 | 537.9756 | 538.96 | 0.0018 |
| K ¹¹⁺ | 19 | 0.05302 | 0.22503 | 0.2597 | 628.7944 | 629.4 | 0.0010 |
| Ca ¹²⁺ | 20 | 0.05035 | 0.21308 | 0.2434 | 726.5442 | 726.6 | 0.0001 |
| Sc ¹³⁺ | 21 | 0.04794 | 0.20235 | 0.2292 | 831.2199 | 830.8 | -0.0005 |
| Ti ¹⁴⁺ | 22 | 0.04574 | 0.19264 | 0.2165 | 942.8179 | 941.9 | -0.0010 |
| V ¹⁵⁺ | 23 | 0.04374 | 0.18383 | 0.2051 | 1061.3351 | 1060 | -0.0013 |
| Cr ¹⁶⁺ | 24 | 0.04191 | 0.17579 | 0.1949 | 1186.7691 | 1185 | -0.0015 |
| Mn ¹⁷⁺ | 25 | 0.04022 | 0.16842 | 0.1857 | 1319.1179 | 1317 | -0.0016 |
| Fe ¹⁸⁺ | 26 | 0.03867 | 0.16165 | 0.1773 | 1458.3799 | 1456 | -0.0016 |
| Co ¹⁹⁺ | 27 | 0.03723 | 0.15540 | 0.1696 | 1604.5538 | 1603 | -0.0010 |
| Ni ²⁰⁺ | 28 | 0.03589 | 0.14961 | 0.1626 | 1757.6383 | 1756 | -0.0009 |
| Cu ²¹⁺ | 29 | 0.03465 | 0.14424 | 0.1561 | 1917.6326 | 1916 | -0.0009 |

^a Radius of the first set of paired inner electrons of eight-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the second set of paired inner electrons of eight-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the two paired and two unpaired outer electrons of eight-electron atoms from Eq. (10.172) (Eq. (64)) for $Z > 8$ and Eq. (10.162) for O .

10 ^d Calculated ionization energies of eight-electron atoms given by the electric energy (Eq. (10.173)) (Eq. (61)).

^e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^f (Experimental-theoretical)/experimental.

TABLE IX. Ionization energies for some nine-electron atoms.

| 9 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_9 (a_0) ^c | Theoretical Ionization Energies ^d (eV) | Experimen- tal Ionization Energies ^e (eV) | Relative Error ^f |
|--------------------------|----|---------------------------------|---------------------------------|---------------------------------|--|--|--------------------------------|
| <i>F</i> | 9 | 0.11297 | 0.51382 | 0.78069 | 17.42782 | 17.42282 | -0.0003 |
| <i>Ne</i> ⁺ | 10 | 0.10149 | 0.45511 | 0.64771 | 42.0121 | 40.96328 | -0.0256 |
| <i>Na</i> ²⁺ | 11 | 0.09213 | 0.40853 | 0.57282 | 71.2573 | 71.62 | 0.0051 |
| <i>Mg</i> ³⁺ | 12 | 0.08435 | 0.37065 | 0.50274 | 108.2522 | 109.2655 | 0.0093 |
| <i>Al</i> ⁴⁺ | 13 | 0.07778 | 0.33923 | 0.44595 | 152.5469 | 153.825 | 0.0083 |
| <i>Si</i> ⁵⁺ | 14 | 0.07216 | 0.31274 | 0.40020 | 203.9865 | 205.27 | 0.0063 |
| <i>P</i> ⁶⁺ | 15 | 0.06730 | 0.29010 | 0.36283 | 262.4940 | 263.57 | 0.0041 |
| <i>S</i> ⁷⁺ | 16 | 0.06306 | 0.27053 | 0.33182 | 328.0238 | 328.75 | 0.0022 |
| <i>Cl</i> ⁸⁺ | 17 | 0.05932 | 0.25344 | 0.30571 | 400.5466 | 400.06 | -0.0012 |
| <i>Ar</i> ⁹⁺ | 18 | 0.05599 | 0.23839 | 0.28343 | 480.0424 | 478.69 | -0.0028 |
| <i>K</i> ¹⁰⁺ | 19 | 0.05302 | 0.22503 | 0.26419 | 566.4968 | 564.7 | -0.0032 |
| <i>Ca</i> ¹¹⁺ | 20 | 0.05035 | 0.21308 | 0.24742 | 659.8992 | 657.2 | -0.0041 |
| <i>Sc</i> ¹²⁺ | 21 | 0.04794 | 0.20235 | 0.23266 | 760.2415 | 756.7 | -0.0047 |
| <i>Ti</i> ¹³⁺ | 22 | 0.04574 | 0.19264 | 0.21957 | 867.5176 | 863.1 | -0.0051 |
| <i>V</i> ¹⁴⁺ | 23 | 0.04374 | 0.18383 | 0.20789 | 981.7224 | 976 | -0.0059 |
| <i>Cr</i> ¹⁵⁺ | 24 | 0.04191 | 0.17579 | 0.19739 | 1102.8523 | 1097 | -0.0053 |
| <i>Mn</i> ¹⁶⁺ | 25 | 0.04022 | 0.16842 | 0.18791 | 1230.9038 | 1224 | -0.0056 |
| <i>Fe</i> ¹⁷⁺ | 26 | 0.03867 | 0.16165 | 0.17930 | 1365.8746 | 1358 | -0.0058 |
| <i>Co</i> ¹⁸⁺ | 27 | 0.03723 | 0.15540 | 0.17145 | 1507.7624 | 1504.6 | -0.0021 |
| <i>Ni</i> ¹⁹⁺ | 28 | 0.03589 | 0.14961 | 0.16427 | 1656.5654 | 1648 | -0.0052 |
| <i>Cu</i> ²⁰⁺ | 29 | 0.03465 | 0.14424 | 0.15766 | 1812.2821 | 1804 | -0.0046 |

^a Radius of the first set of paired inner electrons of nine-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the second set of paired inner electrons of nine-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the one unpaired and two sets of paired outer electrons of nine-electron atoms from Eq. (10.192) (Eq. (64)) for $Z > 9$ and Eq. (10.182) for F .

10 ^d Calculated ionization energies of nine-electron atoms given by the electric energy (Eq. (10.193)) (Eq. (61)).

^e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^f (Experimental-theoretical)/experimental.

TABLE X. Ionization energies for some ten-electron atoms.

| 10 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_{10} (a_0) ^c | Theoretical Ionization Energies ^d (eV) | Experimen tal Ionization Energies ^e (eV) | Relative Error ^f |
|--------------------------|----|---------------------------------|---------------------------------|------------------------------------|--|---|--------------------------------|
| <i>Ne</i> | 10 | 0.10149 | 0.45511 | 0.63659 | 21.37296 | 21.56454 | 0.00888 |
| <i>Na</i> ⁺ | 11 | 0.09213 | 0.40853 | 0.560945 | 48.5103 | 47.2864 | -0.0259 |
| <i>Mg</i> ²⁺ | 12 | 0.08435 | 0.37065 | 0.510568 | 79.9451 | 80.1437 | 0.0025 |
| <i>Al</i> ³⁺ | 13 | 0.07778 | 0.33923 | 0.456203 | 119.2960 | 119.992 | 0.0058 |
| <i>Si</i> ⁴⁺ | 14 | 0.07216 | 0.31274 | 0.409776 | 166.0150 | 166.767 | 0.0045 |
| <i>P</i> ⁵⁺ | 15 | 0.06730 | 0.29010 | 0.371201 | 219.9211 | 220.421 | 0.0023 |
| <i>S</i> ⁶⁺ | 16 | 0.06306 | 0.27053 | 0.339025 | 280.9252 | 280.948 | 0.0001 |
| <i>Cl</i> ⁷⁺ | 17 | 0.05932 | 0.25344 | 0.311903 | 348.9750 | 348.28 | -0.0020 |
| <i>Ar</i> ⁸⁺ | 18 | 0.05599 | 0.23839 | 0.288778 | 424.0365 | 422.45 | -0.0038 |
| <i>K</i> ⁹⁺ | 19 | 0.05302 | 0.22503 | 0.268844 | 506.0861 | 503.8 | -0.0045 |
| <i>Ca</i> ¹⁰⁺ | 20 | 0.05035 | 0.21308 | 0.251491 | 595.1070 | 591.9 | -0.0054 |
| <i>Sc</i> ¹¹⁺ | 21 | 0.04794 | 0.20235 | 0.236251 | 691.0866 | 687.36 | -0.0054 |
| <i>Ti</i> ¹²⁺ | 22 | 0.04574 | 0.19264 | 0.222761 | 794.0151 | 787.84 | -0.0078 |
| <i>V</i> ¹³⁺ | 23 | 0.04374 | 0.18383 | 0.210736 | 903.8853 | 896 | -0.0088 |
| <i>Cr</i> ¹⁴⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 1020.6910 | 1010.6 | -0.0100 |
| <i>Mn</i> ¹⁵⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 1144.4276 | 1134.7 | -0.0086 |
| <i>Fe</i> ¹⁶⁺ | 26 | 0.03867 | 0.16165 | 0.181398 | 1275.0911 | 1266 | -0.0072 |
| <i>Co</i> ¹⁷⁺ | 27 | 0.03723 | 0.15540 | 0.173362 | 1412.6783 | 1397.2 | -0.0111 |
| <i>Ni</i> ¹⁸⁺ | 28 | 0.03589 | 0.14961 | 0.166011 | 1557.1867 | 1541 | -0.0105 |
| <i>Cu</i> ¹⁹⁺ | 29 | 0.03465 | 0.14424 | 0.159261 | 1708.6139 | 1697 | -0.0068 |
| <i>Zn</i> ²⁰⁺ | 30 | 0.03349 | 0.13925 | 0.153041 | 1866.9581 | 1856 | -0.0059 |

^a Radius of the first set of paired inner electrons of ten-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the second set of paired inner electrons of ten-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of three sets of paired outer electrons of ten-electron atoms from Eq. (10.212) (Eq. (64)) for $Z > 10$ and Eq. (10.202) for *Ne*.

10 ^d Calculated ionization energies of ten-electron atoms given by the electric energy (Eq. (10.213)) (Eq. (61)).

^e From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^f (Experimental-theoretical)/experimental.

TABLE XI. Ionization energies for some eleven-electron atoms.

| 11 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | r_{10} (a_0) c | r_{11} (a_0) d | Theoretical Ionization Energies e (eV) | Experimental Ionization Energies f (eV) | Relative Error g |
|-------------------|----|----------------------|----------------------|-------------------------|-------------------------|---|--|---------------------|
| Na | 11 | 0.09213 | 0.40853 | 0.560945 | 2.65432 | 5.12592 | 5.13908 | 0.0026 |
| Mg ⁺ | 12 | 0.08435 | 0.37065 | 0.510568 | 1.74604 | 15.5848 | 15.03528 | -0.0365 |
| Al ²⁺ | 13 | 0.07778 | 0.33923 | 0.456203 | 1.47399 | 27.6918 | 28.44765 | 0.0266 |
| Si ³⁺ | 14 | 0.07216 | 0.31274 | 0.409776 | 1.25508 | 43.3624 | 45.14181 | 0.0394 |
| P ⁴⁺ | 15 | 0.06730 | 0.29010 | 0.371201 | 1.08969 | 62.4299 | 65.0251 | 0.0399 |
| S ⁵⁺ | 16 | 0.06306 | 0.27053 | 0.339025 | 0.96226 | 84.8362 | 88.0530 | 0.0365 |
| Cl ⁶⁺ | 17 | 0.05932 | 0.25344 | 0.311903 | 0.86151 | 110.5514 | 114.1958 | 0.0319 |
| Ar ⁷⁺ | 18 | 0.05599 | 0.23839 | 0.288778 | 0.77994 | 139.5577 | 143.460 | 0.0272 |
| K ⁸⁺ | 19 | 0.05302 | 0.22503 | 0.268844 | 0.71258 | 171.8433 | 175.8174 | 0.0226 |
| Ca ⁹⁺ | 20 | 0.05035 | 0.21308 | 0.251491 | 0.65602 | 207.3998 | 211.275 | 0.0183 |
| Sc ¹⁰⁺ | 21 | 0.04794 | 0.20235 | 0.236251 | 0.60784 | 246.2213 | 249.798 | 0.0143 |
| Ti ¹¹⁺ | 22 | 0.04574 | 0.19264 | 0.222761 | 0.56631 | 288.3032 | 291.500 | 0.0110 |
| V ¹²⁺ | 23 | 0.04374 | 0.18383 | 0.210736 | 0.53014 | 333.6420 | 336.277 | 0.0078 |
| Cr ¹³⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49834 | 382.2350 | 384.168 | 0.0050 |
| Mn ¹⁴⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.47016 | 434.0801 | 435.163 | 0.0025 |
| Fe ¹⁵⁺ | 26 | 0.03867 | 0.16165 | 0.181398 | 0.44502 | 489.1753 | 489.256 | 0.0002 |
| Co ¹⁶⁺ | 27 | 0.03723 | 0.15540 | 0.173362 | 0.42245 | 547.5194 | 546.58 | -0.0017 |
| Ni ¹⁷⁺ | 28 | 0.03589 | 0.14961 | 0.166011 | 0.40207 | 609.1111 | 607.06 | -0.0034 |
| Cu ¹⁸⁺ | 29 | 0.03465 | 0.14424 | 0.159261 | 0.38358 | 673.9495 | 670.588 | -0.0050 |
| Zn ¹⁹⁺ | 30 | 0.03349 | 0.13925 | 0.153041 | 0.36672 | 742.0336 | 738 | -0.0055 |

a Radius of the first set of paired inner electrons of eleven-electron atoms from Eq. (10.51) (Eq. (60)).

5 b Radius of the second set of paired inner electrons of eleven-electron atoms from Eq. (10.62) (Eq. (60)).

c Radius of three sets of paired inner electrons of eleven-electron atoms from Eq. (10.212) (Eq. (64)).

10 d Radius of unpaired outer electron of eleven-electron atoms from Eq. (10.235) (Eq. (60)) for $Z > 11$ and Eq. (10.226) for Na.

e Calculated ionization energies of eleven-electron atoms given by the electric energy (Eq. (10.236)) (Eq. (61)).

f From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

15 g (Experimental-theoretical)/experimental.

TABLE XII. Ionization energies for some twelve-electron atoms.

| 12 e Atom | Z | r_1 (a_o) a | r_3 (a_o) b | r_{10} (a_o) c | r_{12} (a_o) d | Theoretical Ionization Energies e (eV) | Experimental Ionization Energies f (eV) | Relative Error g |
|--------------------------|----|----------------------|----------------------|-------------------------|-------------------------|---|--|---------------------|
| <i>Mg</i> | 12 | 0.08435 | 0.37065 | 0.51057 | 1.79386 | 7.58467 | 7.64624 | 0.0081 |
| <i>Al</i> ⁺ | 13 | 0.07778 | 0.33923 | 0.45620 | 1.41133 | 19.2808 | 18.82856 | -0.0240 |
| <i>Si</i> ²⁺ | 14 | 0.07216 | 0.31274 | 0.40978 | 1.25155 | 32.6134 | 33.49302 | 0.0263 |
| <i>P</i> ³⁺ | 15 | 0.06730 | 0.29010 | 0.37120 | 1.09443 | 49.7274 | 51.4439 | 0.0334 |
| <i>S</i> ⁴⁺ | 16 | 0.06306 | 0.27053 | 0.33902 | 0.96729 | 70.3296 | 72.5945 | 0.0312 |
| <i>Cl</i> ⁵⁺ | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 94.3266 | 97.03 | 0.0279 |
| <i>Ar</i> ⁶⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 121.6724 | 124.323 | 0.0213 |
| <i>K</i> ⁷⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 152.3396 | 154.88 | 0.0164 |
| <i>Ca</i> ⁸⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 186.3102 | 188.54 | 0.0118 |
| <i>Sc</i> ⁹⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 223.5713 | 225.18 | 0.0071 |
| <i>Ti</i> ¹⁰⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 264.1138 | 265.07 | 0.0036 |
| <i>V</i> ¹¹⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 307.9304 | 308.1 | 0.0006 |
| <i>Cr</i> ¹²⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 355.0157 | 354.8 | -0.0006 |
| <i>Mn</i> ¹³⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 405.3653 | 403.0 | -0.0059 |
| <i>Fe</i> ¹⁴⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 458.9758 | 457 | -0.0043 |
| <i>Co</i> ¹⁵⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 515.8442 | 511.96 | -0.0076 |
| <i>Ni</i> ¹⁶⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 575.9683 | 571.08 | -0.0086 |
| <i>Cu</i> ¹⁷⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 639.3460 | 633 | -0.0100 |
| <i>Zn</i> ¹⁸⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 705.9758 | 698 | -0.0114 |

a Radius of the first set of paired inner electrons of twelve-electron atoms from Eq. (10.51) (Eq. (60)).

5 b Radius of the second set of paired inner electrons of twelve-electron atoms from Eq. (10.62) (Eq. (60)).

c Radius of three sets of paired inner electrons of twelve-electron atoms from Eq. (10.212) (Eq. (64)).

d Radius of paired outer electrons of twelve-electron atoms from Eq. (10.255) (Eq. (60)) for $Z > 12$ and Eq. (10.246) for *Mg*.

e Calculated ionization energies of twelve-electron atoms given by the electric energy (Eq. (10.256)) (Eq. (61)).

f From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

15 g (Experimental-theoretical)/experimental.

TABLE XIII. Ionization energies for some thirteen-electron atoms.

| 13 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_{10} (a_0) ^c | r_{12} (a_0) ^d | r_{13} (a_0) ^e | Theoretical Ionization Energies ^f (eV) | Experimental Ionization Energies ^g (eV) | Relative Error ^h |
|--------------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| <i>Al</i> | 13 | 0.07778 | 0.33923 | 0.45620 | 1.41133 | 2.28565 | 5.98402 | 5.98577 | 0.0003 |
| <i>Si</i> ⁺ | 14 | 0.07216 | 0.31274 | 0.40978 | 1.25155 | 1.5995 | 17.0127 | 16.34585 | -0.0408 |
| <i>P</i> ²⁺ | 15 | 0.06730 | 0.29010 | 0.37120 | 1.09443 | 1.3922 | 29.3195 | 30.2027 | 0.0292 |
| <i>S</i> ³⁺ | 16 | 0.06306 | 0.27053 | 0.33902 | 0.96729 | 1.1991 | 45.3861 | 47.222 | 0.0389 |
| <i>Cl</i> ⁴⁺ | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 1.0473 | 64.9574 | 67.8 | 0.0419 |
| <i>Ar</i> ⁵⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 0.9282 | 87.9522 | 91.009 | 0.0336 |
| <i>K</i> ⁶⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.8330 | 114.3301 | 117.56 | 0.0275 |
| <i>Ca</i> ⁷⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.7555 | 144.0664 | 147.24 | 0.0216 |
| <i>Sc</i> ⁸⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.6913 | 177.1443 | 180.03 | 0.0160 |
| <i>Ti</i> ⁹⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.6371 | 213.5521 | 215.92 | 0.0110 |
| <i>V</i> ¹⁰⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.5909 | 253.2806 | 255.7 | 0.0095 |
| <i>Cr</i> ¹¹⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.5510 | 296.3231 | 298.0 | 0.0056 |
| <i>Mn</i> ¹²⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.5162 | 342.6741 | 343.6 | 0.0027 |
| <i>Fe</i> ¹³⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.4855 | 392.3293 | 392.2 | -0.0003 |
| <i>Co</i> ¹⁴⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.4583 | 445.2849 | 444 | -0.0029 |
| <i>Ni</i> ¹⁵⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.4341 | 501.5382 | 499 | -0.0051 |
| <i>Cu</i> ¹⁶⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.4122 | 561.0867 | 557 | -0.0073 |
| <i>Zn</i> ¹⁷⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.3925 | 623.9282 | 619 | -0.0080 |

^a Radius of the paired 1s inner electrons of thirteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of thirteen-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of thirteen-electron atoms from Eq. (10.212)) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of thirteen-electron atoms from Eq. (10.255)) (Eq. (60)).

^e Radius of the unpaired 3p outer electron of thirteen-electron atoms from Eq. (10.288) (Eq. (67)) for $Z > 13$ and Eq. (10.276) for *Al*.

^f Calculated ionization energies of thirteen-electron atoms given by the electric energy (Eq. (10.289)) (Eq. (61)) for $Z > 13$ and Eq. (10.279) for *Al*.

15 ^g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^h (Experimental-theoretical)/experimental.

TABLE XIV. Ionization energies for some fourteen-electron atoms.

| 14 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_{10} (a_0) ^c | r_{12} (a_0) ^d | r_{14} (a_0) ^e | Theoretical Ionization Energies ^f (eV) | Experimental Ionization Energies ^g (eV) | Relative Error ^h |
|-------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| Si | 14 | 0.07216 | 0.31274 | 0.40978 | 1.25155 | 1.67685 | 8.11391 | 8.15169 | 0.0046 |
| P ⁺ | 15 | 0.06730 | 0.29010 | 0.37120 | 1.09443 | 1.35682 | 20.0555 | 19.7694 | -0.0145 |
| S ²⁺ | 16 | 0.06306 | 0.27053 | 0.33902 | 0.96729 | 1.21534 | 33.5852 | 34.790 | 0.0346 |
| Cl ³⁺ | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 1.06623 | 51.0426 | 53.4652 | 0.0453 |
| Ar ⁴⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 0.94341 | 72.1094 | 75.020 | 0.0388 |
| K ⁵⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.84432 | 96.6876 | 99.4 | 0.0273 |
| Ca ⁶⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.76358 | 124.7293 | 127.2 | 0.0194 |
| Sc ⁷⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.69682 | 156.2056 | 158.1 | 0.0120 |
| Ti ⁸⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.64078 | 191.0973 | 192.10 | 0.0052 |
| V ⁹⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.59313 | 229.3905 | 230.5 | 0.0048 |
| Cr ¹⁰⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.55211 | 271.0748 | 270.8 | -0.0010 |
| Mn ¹¹⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.51644 | 316.1422 | 314.4 | -0.0055 |
| Fe ¹²⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.48514 | 364.5863 | 361 | -0.0099 |
| Co ¹³⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.45745 | 416.4021 | 411 | -0.0131 |
| Ni ¹⁴⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.43277 | 471.5854 | 464 | -0.0163 |
| Cu ¹⁵⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.41064 | 530.1326 | 520 | -0.0195 |
| Zn ¹⁶⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.39068 | 592.0410 | 579 | -0.0225 |

^a Radius of the paired 1s inner electrons of fourteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of fourteen-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of fourteen-electron atoms from Eq. (10.212) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of fourteen-electron atoms from Eq. (10.255) (Eq. (60)).

^e Radius of the two unpaired 3p outer electrons of fourteen-electron atoms from Eq. (10.309) (Eq. (67)) for $Z > 14$ and Eq. (10.297) for Si.

^f Calculated ionization energies of fourteen-electron atoms given by the electric energy (Eq. (10.310)) (Eq. (61)).

15 ^g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^h (Experimental-theoretical)/experimental.

TABLE XV. Ionization energies for some fifteen-electron atoms.

| 15 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_{10} (a_0) ^c | r_{12} (a_0) ^d | r_{15} (a_0) ^e | Theoretical Ionization Energies ^f (eV) | Experimental Ionization Energies ^g (eV) | Relative Error ^h |
|--------------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| <i>P</i> | 15 | 0.06730 | 0.29010 | 0.37120 | 1.09443 | 1.28900 | 10.55536 | 10.48669 | -0.0065 |
| <i>S</i> ⁺ | 16 | 0.06306 | 0.27053 | 0.33902 | 0.96729 | 1.15744 | 23.5102 | 23.3379 | -0.0074 |
| <i>Cl</i> ²⁺ | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 1.06759 | 38.2331 | 39.61 | 0.0348 |
| <i>Ar</i> ³⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 0.95423 | 57.0335 | 59.81 | 0.0464 |
| <i>K</i> ⁴⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.85555 | 79.5147 | 82.66 | 0.0381 |
| <i>Ca</i> ⁵⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.77337 | 105.5576 | 108.78 | 0.0296 |
| <i>Sc</i> ⁶⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.70494 | 135.1046 | 138.0 | 0.0210 |
| <i>Ti</i> ⁷⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.64743 | 168.1215 | 170.4 | 0.0134 |
| <i>V</i> ⁸⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.59854 | 204.5855 | 205.8 | 0.0059 |
| <i>Cr</i> ⁹⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.55652 | 244.4799 | 244.4 | -0.0003 |
| <i>Mn</i> ¹⁰⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.52004 | 287.7926 | 286.0 | -0.0063 |
| <i>Fe</i> ¹¹⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.48808 | 334.5138 | 330.8 | -0.0112 |
| <i>Co</i> ¹²⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.45985 | 384.6359 | 379 | -0.0149 |
| <i>Ni</i> ¹³⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.43474 | 438.1529 | 430 | -0.0190 |
| <i>Cu</i> ¹⁴⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.41225 | 495.0596 | 484 | -0.0229 |
| <i>Zn</i> ¹⁵⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.39199 | 555.3519 | 542 | -0.0246 |

^a Radius of the paired 1s inner electrons of fifteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of fifteen-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of fifteen-electron atoms from Eq. (10.212)) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of fifteen-electron atoms from Eq. (10.255)) (Eq. (60)).

^e Radius of the three unpaired 3p outer electrons of fifteen-electron atoms from Eq. (10.331) (Eq. (67)) for $Z > 15$ and Eq. (10.319) for P .

^f Calculated ionization energies of fifteen-electron atoms given by the electric energy (Eq. (10.332)) (Eq. (61)).

15 ^g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^h (Experimental-theoretical)/experimental.

TABLE XVI. Ionization energies for some sixteen-electron atoms.

| 16 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | r_{10} (a_0) c | r_{12} (a_0) d | r_{16} (a_0) e | Theoretical Ionization Energies f (eV) | Experimental Ionization Energies g (eV) | Relative Error h |
|-------------------|----|----------------------|----------------------|-------------------------|-------------------------|-------------------------|---|--|---------------------|
| S | 16 | 0.06306 | 0.27053 | 0.33902 | 0.96729 | 1.32010 | 10.30666 | 10.36001 | 0.0051 |
| Cl ⁺ | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 1.10676 | 24.5868 | 23.814 | -0.0324 |
| Ar ²⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 1.02543 | 39.8051 | 40.74 | 0.0229 |
| K ³⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.92041 | 59.1294 | 60.91 | 0.0292 |
| Ca ⁴⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.82819 | 82.1422 | 84.50 | 0.0279 |
| Sc ⁵⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.75090 | 108.7161 | 110.68 | 0.0177 |
| Ti ⁶⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.68622 | 138.7896 | 140.8 | 0.0143 |
| V ⁷⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.63163 | 172.3256 | 173.4 | 0.0062 |
| Cr ⁸⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.58506 | 209.2996 | 209.3 | 0.0000 |
| Mn ⁹⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.54490 | 249.6938 | 248.3 | -0.0056 |
| Fe ¹⁰⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.50994 | 293.4952 | 290.2 | -0.0114 |
| Co ¹¹⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.47923 | 340.6933 | 336 | -0.0140 |
| Ni ¹²⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.45204 | 391.2802 | 384 | -0.0190 |
| Cu ¹³⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.42781 | 445.2492 | 435 | -0.0236 |
| Zn ¹⁴⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.40607 | 502.5950 | 490 | -0.0257 |

a Radius of the paired 1s inner electrons of sixteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 b Radius of the paired 2s inner electrons of sixteen-electron atoms from Eq. (10.62) (Eq. (60)).

c Radius of the three sets of paired 2p inner electrons of sixteen-electron atoms from Eq. (10.212) (Eq. (64)).

10 d Radius of the paired 3s inner electrons of sixteen-electron atoms from Eq. (10.255) (Eq. (60)).

e Radius of the two paired and two unpaired 3p outer electrons of sixteen-electron atoms from Eq. (10.353) (Eq. (67)) for $Z > 16$ and Eq. (10.341) for S.

f Calculated ionization energies of sixteen-electron atoms given by the electric energy (Eq. (10.354)) (Eq. (61)).

15 g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

h (Experimental-theoretical)/experimental.

TABLE XVII. Ionization energies for some seventeen-electron atoms.

| 17 e Atom | Z | r_1 (a_0) a | r_3 (a_0) b | r_{10} (a_0) c | r_{12} (a_0) d | r_{17} (a_0) e | Theoretical Ionization Energies f (eV) | Experimental Ionization Energies g (eV) | Relative Error h |
|-------------------|----|----------------------|----------------------|-------------------------|-------------------------|-------------------------|---|--|---------------------|
| Cl | 17 | 0.05932 | 0.25344 | 0.31190 | 0.86545 | 1.05158 | 12.93841 | 12.96764 | 0.0023 |
| Ar ⁺ | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 0.98541 | 27.6146 | 27.62967 | 0.0005 |
| K ²⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.93190 | 43.8001 | 45.806 | 0.0438 |
| Ca ³⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.84781 | 64.1927 | 67.27 | 0.0457 |
| Sc ⁴⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.77036 | 88.3080 | 91.65 | 0.0365 |
| Ti ⁵⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.70374 | 116.0008 | 119.53 | 0.0295 |
| V ⁶⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.64701 | 147.2011 | 150.6 | 0.0226 |
| Cr ⁷⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.59849 | 181.8674 | 184.7 | 0.0153 |
| Mn ⁸⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.55667 | 219.9718 | 221.8 | 0.0082 |
| Fe ⁹⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.52031 | 261.4942 | 262.1 | 0.0023 |
| Co ¹⁰⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.48843 | 306.4195 | 305 | -0.0047 |
| Ni ¹¹⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.46026 | 354.7360 | 352 | -0.0078 |
| Cu ¹²⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.43519 | 406.4345 | 401 | -0.0136 |
| Zn ¹³⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.41274 | 461.5074 | 454 | -0.0165 |

a Radius of the paired 1s inner electrons of seventeen-electron atoms from Eq. (10.51) (Eq. (60)).

5 b Radius of the paired 2s inner electrons of seventeen-electron atoms from Eq. (10.62) (Eq. (60)).

c Radius of the three sets of paired 2p inner electrons of seventeen-electron atoms from Eq. (10.212) (Eq. (64)).

10 d Radius of the paired 3s inner electrons of seventeen-electron atoms from Eq. (10.255) (Eq. (60)).

e Radius of the two sets of paired and an unpaired 3p outer electron of seventeen-electron atoms from Eq. (10.376) (Eq. (67)) for $Z > 17$ and Eq. (10.363) for Cl.

f Calculated ionization energies of seventeen-electron atoms given by the electric energy (Eq. (10.377)) (Eq. (61)).

15 g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

h (Experimental-theoretical)/experimental.

TABLE XVIII. Ionization energies for some eighteen-electron atoms.

| 18 e Atom | Z | r_1 (a_o) ^a | r_3 (a_o) ^b | r_{10} (a_o) ^c | r_{12} (a_o) ^d | r_{18} (a_o) ^e | Theoretical Ionization Energies ^f (eV) | Experimental Ionization Energies ^g (eV) | Relative Error ^h |
|--------------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| <i>Ar</i> | 18 | 0.05599 | 0.23839 | 0.28878 | 0.78276 | 0.86680 | 15.69651 | 15.75962 | 0.0040 |
| <i>K</i> ⁺ | 19 | 0.05302 | 0.22503 | 0.26884 | 0.71450 | 0.85215 | 31.9330 | 31.63 | -0.0096 |
| <i>Ca</i> ²⁺ | 20 | 0.05035 | 0.21308 | 0.25149 | 0.65725 | 0.82478 | 49.4886 | 50.9131 | 0.0280 |
| <i>Sc</i> ³⁺ | 21 | 0.04794 | 0.20235 | 0.23625 | 0.60857 | 0.76196 | 71.4251 | 73.4894 | 0.0281 |
| <i>Ti</i> ⁴⁺ | 22 | 0.04574 | 0.19264 | 0.22276 | 0.56666 | 0.70013 | 97.1660 | 99.30 | 0.0215 |
| <i>V</i> ⁵⁺ | 23 | 0.04374 | 0.18383 | 0.21074 | 0.53022 | 0.64511 | 126.5449 | 128.13 | 0.0124 |
| <i>Cr</i> ⁶⁺ | 24 | 0.04191 | 0.17579 | 0.19995 | 0.49822 | 0.59718 | 159.4836 | 160.18 | 0.0043 |
| <i>Mn</i> ⁷⁺ | 25 | 0.04022 | 0.16842 | 0.19022 | 0.46990 | 0.55552 | 195.9359 | 194.5 | -0.0074 |
| <i>Fe</i> ⁸⁺ | 26 | 0.03867 | 0.16165 | 0.18140 | 0.44466 | 0.51915 | 235.8711 | 233.6 | -0.0097 |
| <i>Co</i> ⁹⁺ | 27 | 0.03723 | 0.15540 | 0.17336 | 0.42201 | 0.48720 | 279.2670 | 275.4 | -0.0140 |
| <i>Ni</i> ¹⁰⁺ | 28 | 0.03589 | 0.14961 | 0.16601 | 0.40158 | 0.45894 | 326.1070 | 321.0 | -0.0159 |
| <i>Cu</i> ¹¹⁺ | 29 | 0.03465 | 0.14424 | 0.15926 | 0.38305 | 0.43379 | 376.3783 | 369 | -0.0200 |
| <i>Zn</i> ¹²⁺ | 30 | 0.03349 | 0.13925 | 0.15304 | 0.36617 | 0.41127 | 430.0704 | 419.7 | -0.0247 |

^a Radius of the paired 1s inner electrons of eighteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of eighteen-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of eighteen-electron atoms from Eq. (10.212) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of eighteen-electron atoms from Eq. (10.255) (Eq. (60)).

^e Radius of the three sets of paired 3p outer electrons of eighteen-electron atoms from Eq. (10.399) (Eq. (67)) for $Z > 18$ and Eq. (10.386) for *Ar*.

^f Calculated ionization energies of eighteen-electron atoms given by the electric energy (Eq. (10.400)) (Eq. (61)).

15 ^g From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

^h (Experimental-theoretical)/experimental.

TABLE XIX. Ionization energies for some nineteen-electron atoms.

| 19 e Atom | Z | r_1 (a_o) ^a | r_3 (a_o) ^b | r_{10} (a_o) ^c | r_{12} (a_o) ^d | r_{18} (a_o) ^e | r_{19} (a_o) ^f | Theoretical Ionization Energies ^g (eV) | Experimental Ionization Energies ^h (eV) | Relative Error ⁱ |
|--------------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| <i>K</i> | 19 | 0.053 02 | 0.225 03 | 0.268 84 | 0.714 50 | 0.852 15 | 3.145 15 | 4.32596 | 4.34066 | 0.0034 |
| <i>Ca</i> ⁺ | 20 | 0.050 35 | 0.213 08 | 0.251 49 | 0.657 25 | 0.824 78 | 2.400 60 | 11.3354 | 11.87172 | 0.0452 |
| <i>Sc</i> ²⁺ | 21 | 0.047 94 | 0.202 35 | 0.236 25 | 0.608 57 | 0.761 96 | 1.652 61 | 24.6988 | 24.75666 | 0.0023 |
| <i>Ti</i> ³⁺ | 22 | 0.045 74 | 0.192 64 | 0.222 76 | 0.566 66 | 0.700 13 | 1.299 98 | 41.8647 | 43.2672 | 0.0324 |
| <i>V</i> ⁴⁺ | 23 | 0.043 74 | 0.183 83 | 0.210 74 | 0.530 22 | 0.645 11 | 1.082 45 | 62.8474 | 65.2817 | 0.0373 |
| <i>Cr</i> ⁵⁺ | 24 | 0.041 91 | 0.175 79 | 0.199 95 | 0.498 22 | 0.597 18 | 0.931 56 | 87.6329 | 90.6349 | 0.0331 |
| <i>Mn</i> ⁶⁺ | 25 | 0.040 22 | 0.168 42 | 0.190 22 | 0.469 90 | 0.555 52 | 0.819 57 | 116.2076 | 119.203 | 0.0251 |
| <i>Fe</i> ⁷⁺ | 26 | 0.038 67 | 0.161 65 | 0.181 40 | 0.444 66 | 0.519 15 | 0.732 67 | 148.5612 | 151.06 | 0.0165 |
| <i>Co</i> ⁸⁺ | 27 | 0.037 23 | 0.155 40 | 0.173 36 | 0.422 01 | 0.487 20 | 0.663 03 | 184.6863 | 186.13 | 0.0078 |
| <i>Ni</i> ⁹⁺ | 28 | 0.035 89 | 0.149 61 | 0.166 01 | 0.401 58 | 0.458 94 | 0.605 84 | 224.5772 | 224.6 | 0.0001 |
| <i>Cu</i> ¹⁰⁺ | 29 | 0.034 65 | 0.144 24 | 0.159 26 | 0.383 05 | 0.433 79 | 0.557 97 | 268.2300 | 265.3 | -0.0110 |
| <i>Zn</i> ¹¹⁺ | 30 | 0.033 49 | 0.139 25 | 0.153 04 | 0.366 17 | 0.411 27 | 0.517 26 | 315.6418 | 310.8 | -0.0156 |

^a Radius of the paired 1s inner electrons of nineteen-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of nineteen-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of nineteen-electron atoms from Eq. (10.212)) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of nineteen-electron atoms from Eq. (10.255)) (Eq. (60)).

^e Radius of the three sets of paired 3p inner electrons of nineteen-electron atoms from Eq. (10.399) (Eq. (67)).

^f Radius of the unpaired 4s outer electron of nineteen-electron atoms from Eq. (10.425) (Eq. (60)) for $Z > 19$ and Eq. (10.414) for *K*.

15 ^g Calculated ionization energies of nineteen-electron atoms given by the electric energy (Eq. (10.426)) (Eq. (61)).

^h From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

ⁱ (Experimental-theoretical)/experimental.

TABLE XX. Ionization energies for some twenty-electron atoms.

| 20 e Atom | Z | r_1 (a_0) ^a | r_3 (a_0) ^b | r_{10} (a_0) ^c | r_{12} (a_0) ^d | r_{18} (a_0) ^e | r_{20} (a_0) ^f | Theoretical Ionization Energies ^g (eV) | Experimental Ionization Energies ^h (eV) | Relative Error ⁱ |
|-------------------|----|---------------------------------|---------------------------------|------------------------------------|------------------------------------|------------------------------------|------------------------------------|--|---|--------------------------------|
| Ca | 20 | 0.050 35 | 0.213 08 | 0.251 49 | 0.657 25 | 0.824 78 | 2.230 09 | 6.10101 | 6.11316 | 0.0020 |
| Sc ⁺ | 21 | 0.047 94 | 0.202 35 | 0.236 25 | 0.608 57 | 0.761 96 | 2.048 69 | 13.2824 | 12.79967 | -0.0377 |
| Ti ²⁺ | 22 | 0.045 74 | 0.192 64 | 0.222 76 | 0.566 66 | 0.700 13 | 1.485 79 | 27.4719 | 27.4917 | 0.0007 |
| V ³⁺ | 23 | 0.043 74 | 0.183 83 | 0.210 74 | 0.530 22 | 0.645 11 | 1.191 00 | 45.6956 | 46.709 | 0.0217 |
| Cr ⁴⁺ | 24 | 0.041 91 | 0.175 79 | 0.199 95 | 0.498 22 | 0.597 18 | 1.002 20 | 67.8794 | 69.46 | 0.0228 |
| Mn ⁵⁺ | 25 | 0.040 22 | 0.168 42 | 0.190 22 | 0.469 90 | 0.555 52 | 0.868 67 | 93.9766 | 95.6 | 0.0170 |
| Fe ⁶⁺ | 26 | 0.038 67 | 0.161 65 | 0.181 40 | 0.444 66 | 0.519 15 | 0.768 34 | 123.9571 | 124.98 | 0.0082 |
| Co ⁷⁺ | 27 | 0.037 23 | 0.155 40 | 0.173 36 | 0.422 01 | 0.487 20 | 0.689 77 | 157.8012 | 157.8 | 0.0000 |
| Ni ⁸⁺ | 28 | 0.035 89 | 0.149 61 | 0.166 01 | 0.401 58 | 0.458 94 | 0.626 37 | 195.4954 | 193 | -0.0129 |
| Cu ⁹⁺ | 29 | 0.034 65 | 0.144 24 | 0.159 26 | 0.383 05 | 0.433 79 | 0.574 01 | 237.0301 | 232 | -0.0217 |
| Zn ¹⁰⁺ | 30 | 0.033 49 | 0.139 25 | 0.153 04 | 0.366 17 | 0.411 27 | 0.529 97 | 282.3982 | 274 | -0.0307 |

^a Radius of the paired 1s inner electrons of twenty-electron atoms from Eq. (10.51) (Eq. (60)).

5 ^b Radius of the paired 2s inner electrons of twenty-electron atoms from Eq. (10.62) (Eq. (60)).

^c Radius of the three sets of paired 2p inner electrons of twenty-electron atoms from Eq. (10.212)) (Eq. (64)).

10 ^d Radius of the paired 3s inner electrons of twenty-electron atoms from Eq. (10.255)) (Eq. (60)).

^e Radius of the three sets of paired 3p inner electrons of twenty-electron atoms from Eq. (10.399) (Eq. (67)).

^f Radius of the paired 4s outer electrons of twenty-electron atoms from Eq. (10.445) (Eq. (60)) for $Z > 20$ and Eq. (10.436) for Ca.

15 ^g Calculated ionization energies of twenty-electron atoms given by the electric energy (Eq. (10.446)) (Eq. (61)).

^h From theoretical calculations, interpolation of isoelectronic and spectral series, and experimental data [24-25].

ⁱ (Experimental-theoretical)/experimental.

GENERAL EQUATION FOR THE IONIZATION ENERGIES OF ATOMS HAVING AN OUTER S-SHELL

The derivation of the radii and energies of the 1s, 2s, 3s, and 4s electrons is given in the One-Electron Atom, the Two-Electron Atom, the Three-Electron Atoms, the Four-Electron Atoms, the Eleven-Electron Atoms, the Twelve-Electron Atoms, the Nineteen-Electron Atoms, and the Twenty-Electron Atoms sections of Ref. [4]. (Reference to equations of the form Eq. (1.number), Eq. (7.number), and Eq. (10.number) will refer to the corresponding equations of Ref. [4].) The general equation for the radii of s electrons is given by

$$r_n = \frac{a_0 \left(1 + (C - D) \frac{\sqrt{3}}{2Z} \right)}{\left((Z - (n - 1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_m} \right)} \pm a_0 \sqrt{\frac{\left(1 + (C - D) \frac{\sqrt{3}}{2Z} \right)^2}{\left((Z - (n - 1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_m} \right)} + \frac{20\sqrt{3} \left(\left[\frac{Z - n}{Z - (n - 1)} \right] E r_m \right)}{\left((Z - (n - 1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_m} \right)}} \quad (60)$$

r_m in units of a_0

where Z is the nuclear charge, n is the number of electrons, r_m is the radius of the proceeding filled shell(s) given by Eq. (60) for the preceding s shell(s), Eq. (64) for the 2p shell, and Eq. (69) for the 3p shell, the parameter A given in TABLE XXI corresponds to the diamagnetic force, $F_{\text{diamagnetic}}$, (Eq. (10.11)), the parameter B given in TABLE XXI corresponds to the paramagnetic force, $F_{\text{mag}2}$ (Eq. (10.55)), the parameter C given in TABLE XXI corresponds to the diamagnetic force, $F_{\text{diamagnetic}3}$, (Eq. (10.221)), the parameter D given in TABLE XXI corresponds to the paramagnetic force, F_{mag} , (Eq. (7.15)), and the parameter E given in TABLE XXI corresponds to the diamagnetic force, $F_{\text{diamagnetic}2}$, due to a relativistic effect with an electric field for $r > r_n$ (Eqs. (10.35), (10.229), and (10.418)). The positive root of Eq. (60) must be taken in order that $r_n > 0$. The radii of several n-electron atoms having an outer s shell are given in TABLES I-IV, XI-XII, XIX and XX.

The ionization energy for atoms having an outer s-shell are given by the negative of the electric energy, $E(\text{electric})$, (Eq. (10.102) with the radii, r_n , given by Eq. (60) and Eq. (10.447)):

$$E(\text{Ionization}) = -\text{Electric Energy} = \frac{(Z - (n - 1))e^2}{8\pi\epsilon_0 r_n} \quad (61)$$

except that minor corrections due to the magnetic energy must be included in cases wherein the s electron does not couple to p electrons as given in Eqs. (7.28), (7.47), (10.25), (10.48), (10.66), and (10.68). Since the relativistic corrections were small
 5 except for one, two, and three-electron atoms, the nonrelativistic ionization energies for experimentally measured n-electron, s-filling atoms are given in most cases by Eqs. (60) and (61). The ionization energies of several n-electron atoms having an outer s shell are given in TABLES I-IV, XI-XII, XIX and XX.

10 TABLE XXI. Summary of the parameters of atoms filling the 1s, 2s, 3s, and 4s orbitals.

| Atom Type | Electron Configuration | Ground State Term ^a | Orbital Arrangement of s Electrons (s state) | Diam ag. Force Factor A^b | Para mag. Force Factor B^c | Diam ag. Force Factor C^d | Para mag. Force Factor D^e | Diam ag. Force Factor E^f |
|--------------------------------|---------------------------------|--------------------------------|--|-----------------------------|------------------------------|-----------------------------|------------------------------|-----------------------------|
| Neutral 1 e Atom <i>H</i> | $1s^1$ | $^2S_{1/2}$ | \uparrow 1s | 0 | 0 | 0 | 0 | 0 |
| Neutral 2 e Atom <i>He</i> | $1s^2$ | 1S_0 | $\uparrow\downarrow$ 1s | 0 | 0 | 0 | 1 | 0 |
| Neutral 3 e Atom <i>Li</i> | $2s^1$ | $^2S_{1/2}$ | \uparrow 2s | 1 | 0 | 0 | 0 | 0 |
| Neutral 4 e Atom <i>Be</i> | $2s^2$ | 1S_0 | $\uparrow\downarrow$ 2s | 1 | 0 | 0 | 1 | 0 |
| Neutral 11 e Atom <i>Na</i> | $1s^2 2s^2 2p^6 3s^1$ | $^2S_{1/2}$ | \uparrow 3s | 1 | 0 | 8 | 0 | 0 |
| Neutral 12 e Atom <i>Mg</i> | $1s^2 2s^2 2p^6 3s^2$ | 1S_0 | $\uparrow\downarrow$ 3s | 1 | 3 | 12 | 1 | 0 |
| Neutral 19 e Atom <i>K</i> | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ | $^2S_{1/2}$ | \uparrow 4s | 2 | 0 | 12 | 0 | 0 |
| Neutral 20 e Atom <i>Ca</i> | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$ | 1S_0 | $\uparrow\downarrow$ 4s | 1 | 3 | 24 | 1 | 0 |
| 1 e Ion | $1s^1$ | $^2S_{1/2}$ | \uparrow 1s | 0 | 0 | 0 | 0 | 0 |
| 2 e Ion | $1s^2$ | 1S_0 | $\uparrow\downarrow$ 1s | 0 | 0 | 0 | 1 | 0 |
| 3 e Ion | $2s^1$ | $^2S_{1/2}$ | \uparrow 2s | 1 | 0 | 0 | 0 | 1 |
| 4 e Ion | $2s^2$ | 1S_0 | $\uparrow\downarrow$ 2s | 1 | 0 | 0 | 1 | 1 |
| 11 e Ion | $1s^2 2s^2 2p^6 3s^1$ | $^2S_{1/2}$ | \uparrow 3s | 1 | 4 | 8 | 0 | $1 + \frac{\sqrt{2}}{2}$ |

| | | | | | | | | |
|----------|---------------------------------|-------------|--|---|---|----|---|--------------------------|
| 12 e ion | $1s^2 2s^2 2p^6 3s^2$ | 1S_0 | $\begin{array}{c} \uparrow \downarrow \\ 3s \end{array}$ | 1 | 6 | 0 | 0 | $1 + \frac{\sqrt{2}}{2}$ |
| 19 e ion | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ | $^2S_{1/2}$ | $\begin{array}{c} \uparrow \\ 4s \end{array}$ | 3 | 0 | 24 | 0 | $2 - \sqrt{2}$ |
| 20 e ion | $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$ | 1S_0 | $\begin{array}{c} \uparrow \downarrow \\ 4s \end{array}$ | 2 | 0 | 24 | 0 | $2 - \sqrt{2}$ |

a The theoretical ground state terms match those given by NIST [26].

b Eq. (10.11).

c Eq. (10.55).

d Eq. (10.221).

5 e Eq. (7.15).

f Eqs. (10.35), (10.229), and (10.418).

GENERAL EQUATION FOR THE IONIZATION ENERGIES OF FIVE THROUGH TEN-ELECTRON ATOMS

10

The derivation of the radii and energies of the 2p electrons is given in the Five through Eight-Electron Atoms sections of Ref. [4]. Using the forces given by Eqs. (58) (Eq. (10.70)), (10.82-10.84), (10.89), (10.93), and the radii r_3 given by Eq. (10.62) (from Eq. (60)), the radii of the 2p electrons of all five through ten-electron atoms may be solved exactly. The electric energy given by Eq. (61) (Eq. (10.102)) gives the corresponding exact ionization energies. A summary of the parameters of the equations that determine the exact radii and ionization energies of all five through ten-electron atoms is given in TABLE XXII.

15

TABLE XXII. Summary of the parameters of five through ten-electron atoms.

| Atom Type | Electron Configuration | Ground State Term ^a | Orbital Arrangement of 2p Electrons (2p state) | | | Diamagnetic Force Factor A^b | Paramagnetic Force Factor B^c |
|--------------------------------|------------------------|--------------------------------|--|---------------------------|----------------------------|--------------------------------|---------------------------------|
| Neutral 5 e Atom <i>B</i> | $1s^2 2s^2 2p^1$ | $^2P_{1/2}^0$ | \uparrow 1 | — 0 | — -1 | 2 | 0 |
| Neutral 6 e Atom <i>C</i> | $1s^2 2s^2 2p^2$ | 3P_0 | \uparrow 1 | \uparrow 0 | — -1 | $\frac{2}{3}$ | 0 |
| Neutral 7 e Atom <i>N</i> | $1s^2 2s^2 2p^3$ | $^4S_{3/2}^0$ | \uparrow 1 | \uparrow 0 | \uparrow -1 | $\frac{1}{3}$ | 1 |
| Neutral 8 e Atom <i>O</i> | $1s^2 2s^2 2p^4$ | 3P_2 | $\uparrow\downarrow$ 1 | \uparrow 0 | \uparrow -1 | 1 | 2 |
| Neutral 9 e Atom <i>F</i> | $1s^2 2s^2 2p^5$ | $^2P_{3/2}^0$ | $\uparrow\downarrow$ 1 | $\uparrow\downarrow$ 0 | \uparrow -1 | $\frac{2}{3}$ | 3 |
| Neutral 10 e Atom <i>Ne</i> | $1s^2 2s^2 2p^6$ | 1S_0 | $\uparrow\downarrow$ 1 | $\uparrow\downarrow$ 0 | $\uparrow\downarrow$ -1 | 0 | 3 |
| 5 e Ion | $1s^2 2s^2 2p^1$ | $^2P_{1/2}^0$ | \uparrow 1 | — 0 | — -1 | $\frac{5}{3}$ | 1 |
| 6 e Ion | $1s^2 2s^2 2p^2$ | 3P_0 | \uparrow 1 | \uparrow 0 | — -1 | $\frac{5}{3}$ | 4 |
| 7 e Ion | $1s^2 2s^2 2p^3$ | $^4S_{3/2}^0$ | \uparrow 1 | \uparrow 0 | \uparrow -1 | $\frac{5}{3}$ | 6 |
| 8 e Ion | $1s^2 2s^2 2p^4$ | 3P_2 | $\uparrow\downarrow$ 1 | \uparrow 0 | \uparrow -1 | $\frac{5}{3}$ | 6 |
| 9 e Ion | $1s^2 2s^2 2p^5$ | $^2P_{3/2}^0$ | $\uparrow\downarrow$ 1 | $\uparrow\downarrow$ 0 | \uparrow -1 | $\frac{5}{3}$ | 9 |
| 10 e Ion | $1s^2 2s^2 2p^6$ | 1S_0 | $\uparrow\downarrow$ 1 | $\uparrow\downarrow$ 0 | $\uparrow\downarrow$ -1 | $\frac{5}{3}$ | 12 |

^a The theoretical ground state terms match those given by NIST [26].^b Eq. (10.82).^c Eqs. (10.83-10.84) and (10.89).

F_{ele} and $F_{diamagnetic\ 2}$ given by Eqs. (58) (Eq. (10.70)) and (10.93), respectively, are of the same form for all atoms with the appropriate nuclear charges and atomic radii. $F_{diamagnetic}$ given by Eq. (10.82) and $F_{mag\ 2}$ given by Eqs. (10.83-10.84) and (10.89) are of the same form with the appropriate factors that depend on the
 5 electron configuration wherein the electron configuration given in TABLE XXII must be a minimum of energy.

For each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^{n-4}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by Eqs. (7.19) and (10.51) (from Eq. (60)):

$$r_1 = r_2 = a_0 \left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right] \quad (62)$$

two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by Eq. (10.62) (from Eq. (60)):

$$r_4 = r_3 = \frac{\left(a_0 \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right) \right)}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)} \pm a_0 \frac{\left(\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)^2 \right)}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)^2} + 4 \frac{\left[\frac{Z-3}{Z-2} \right] r_1 10 \sqrt{\frac{3}{4}}}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)} \quad (63)$$

r_1 in units of a_0
 15 where r_1 is given by Eq. (62), and $n - 4$ electrons in an orbitsphere with radius r_n given by

$$r_n = \frac{a_0 \left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_3} \right) \pm a_0 \sqrt{\frac{1}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_3} \right)^2} + \frac{20\sqrt{3} \left(\left[\frac{Z-n}{Z-(n-1)} \right] \left(1 - \frac{\sqrt{2}}{2} \right) r_3 \right)}{\left((Z - (n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_3} \right)}}}{2} \quad (64)$$

r_3 in units of a_0

where r_3 is given by Eq. (63), the parameter A given in TABLE XXII corresponds to the diamagnetic force, $F_{\text{diamagnetic}}$, (Eq. (10.82)), and the parameter B given in TABLE XXII corresponds to the paramagnetic force, $F_{\text{mag}2}$ (Eqs. (10.83-10.84) and (10.89)).

- 5 The positive root of Eq. (64) must be taken in order that $r_n > 0$. The radii of several n-electron atoms are given in TABLES V-X.

The ionization energy for the boron atom is given by Eq. (10.104). The ionization energies for the n-electron atoms are given by the negative of the electric energy, $E(\text{electric})$, (Eq. (61) with the radii, r_n , given by Eq. (64)). Since the

10 relativistic corrections were small, the nonrelativistic ionization energies for experimentally measured n-electron atoms are given by Eqs. (61) and (64) in TABLES V-X.

15 GENERAL EQUATION FOR THE IONIZATION ENERGIES OF THIRTEEN THROUGH EIGHTEEN-ELECTRON ATOMS

The derivation of the radii and energies of the 3p electrons is given in the Thirteen through Eighteen-Electron Atoms sections of Ref. [4]. Using the forces given by Eqs. (58) (Eq.(10.257)), (10.258-10.264), (10.268), and the radii r_{12} given

20 by Eq. (10.255) (from Eq. (60)), the radii of the 3p electrons of all thirteen through eighteen-electron atoms may be solved exactly. The electric energy given by Eq. (61) (Eq. (10.102)) gives the corresponding exact ionization energies. A summary of the parameters of the equations that determine the exact radii and ionization energies of all thirteen through eighteen-electron atoms is given in TABLES XIII-

25 XVIII.

F_{ele} and $F_{\text{diamagnetic}2}$ given by Eqs. (58) (Eq. (10.257)) and (10.268), respectively, are of the same form for all atoms with the appropriate nuclear charges

and atomic radii. $F_{\text{diamagnetic}}$ given by Eq. (10.258) and $F_{\text{mag } 2}$ given by Eqs. (10.259-10.264) are of the same form with the appropriate factors that depend on the electron configuration given in TABLE XXIII wherein the electron configuration must be a minimum of energy.

5

TABLE XXIII. Summary of the parameters of thirteen through eighteen-electron atoms.

| Atom Type | Electron Configuration | Ground State Term ^a | Orbital Arrangement of 3p Electrons (3p state) | Diamagnetic Force Factor A^b | Paramagnetic Force Factor B^c |
|--------------------------------|----------------------------|--------------------------------|---|--------------------------------|---------------------------------|
| Neutral 13 e Atom <i>Al</i> | $1s^2 2s^2 2p^6 3s^2 3p^1$ | $^2P_{1/2}^0$ | $\begin{array}{ccc} \uparrow & _ & _ \\ 1 & 0 & -1 \end{array}$ | $\frac{11}{3}$ | 0 |
| Neutral 14 e Atom <i>Si</i> | $1s^2 2s^2 2p^6 3s^2 3p^2$ | 3P_0 | $\begin{array}{ccc} \uparrow & \uparrow & _ \\ 1 & 0 & -1 \end{array}$ | $\frac{7}{3}$ | 0 |
| Neutral 15 e Atom <i>P</i> | $1s^2 2s^2 2p^6 3s^2 3p^3$ | $^4S_{3/2}^0$ | $\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | $\frac{5}{3}$ | 2 |
| Neutral 16 e Atom <i>S</i> | $1s^2 2s^2 2p^6 3s^2 3p^4$ | 3P_2 | $\begin{array}{ccc} \uparrow\downarrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | $\frac{4}{3}$ | 1 |
| Neutral 17 e Atom <i>Cl</i> | $1s^2 2s^2 2p^6 3s^2 3p^5$ | $^2P_{3/2}^0$ | $\begin{array}{ccc} \uparrow\downarrow & \uparrow\downarrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | $\frac{2}{3}$ | 2 |
| Neutral 18 e Atom <i>Ar</i> | $1s^2 2s^2 2p^6 3s^2 3p^6$ | 1S_0 | $\begin{array}{ccc} \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow \\ 1 & 0 & -1 \end{array}$ | $\frac{1}{3}$ | 4 |
| 13 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^1$ | $^2P_{1/2}^0$ | $\begin{array}{ccc} \uparrow & _ & _ \\ 1 & 0 & -1 \end{array}$ | $\frac{5}{3}$ | 12 |
| 14 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^2$ | 3P_0 | $\begin{array}{ccc} \uparrow & \uparrow & _ \\ 1 & 0 & -1 \end{array}$ | $\frac{1}{3}$ | 16 |
| 15 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^3$ | $^4S_{3/2}^0$ | $\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | 0 | 24 |
| 16 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^4$ | 3P_2 | $\begin{array}{ccc} \uparrow\downarrow & \uparrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | $\frac{1}{3}$ | 24 |
| 17 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^5$ | $^2P_{3/2}^0$ | $\begin{array}{ccc} \uparrow\downarrow & \uparrow\downarrow & \uparrow \\ 1 & 0 & -1 \end{array}$ | $\frac{2}{3}$ | 32 |
| 18 e Ion | $1s^2 2s^2 2p^6 3s^2 3p^6$ | 1S_0 | $\begin{array}{ccc} \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow \\ 1 & 0 & -1 \end{array}$ | 0 | 40 |

^a The theoretical ground state terms match those given by NIST [26].

b Eq. (10.258).

c Eqs. (10.260-10.264).

- 5 For each n-electron atom having a central charge of Z times that of the proton and an electron configuration $1s^2 2s^2 2p^6 3s^2 3p^{n-12}$, there are two indistinguishable spin-paired electrons in an orbitsphere with radii r_1 and r_2 both given by Eq. (7.19) and (10.51) (from Eq. (60)):

$$r_1 = r_2 = a_0 \left[\frac{1}{Z-1} - \frac{\sqrt{\frac{3}{4}}}{Z(Z-1)} \right] \quad (65)$$

- 10 two indistinguishable spin-paired electrons in an orbitsphere with radii r_3 and r_4 both given by Eq. (10.62) (from Eq. (60)):

$$r_4 = r_3 = \frac{\left(a_0 \left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right) \right) \left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right) \pm a_0 \sqrt{\frac{\left(\left(1 - \frac{\sqrt{\frac{3}{4}}}{Z} \right)^2 \right) \left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)^2 + 4 \left[\frac{Z-3}{Z-2} \right] r_1^{10} \sqrt{\frac{3}{4}}}}{\left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right) \left((Z-3) - \left(\frac{1}{4} - \frac{1}{Z} \right) \frac{\sqrt{\frac{3}{4}}}{r_1} \right)}} \quad (66)$$

r_1 in units of a_0

where r_1 is given by Eq. (65), three sets of paired indistinguishable electrons in an orbitsphere with radius r_{10} given by Eq. (64) (Eq. (10.212)):

$$r_{10} = \frac{\left(\frac{a_0}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)} \pm a_0 \right)}{2} \sqrt[2]{\frac{1}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)} + \frac{20\sqrt{3} \left(\left[\frac{Z-10}{Z-9} \right] \left(1 - \frac{\sqrt{2}}{2} \right) r_3 \right)}{\left((Z-9) - \left(\frac{5}{24} - \frac{6}{Z} \right) \frac{\sqrt{3}}{r_3} \right)}} \quad (67)$$

r_3 in units of a_0

where r_3 is given by Eq. (66) (Eqs. (10.62) and (10.402)), two indistinguishable spin-paired electrons in an orbitsphere with radius r_{12} given by Eq. (10.255) (from Eq. (60)):

$$r_{12} = \frac{\left(\frac{a_0}{\left((Z-11) - \left(\frac{1}{8} - \frac{3}{Z} \right) \frac{\sqrt{3}}{r_{10}} \right)} \pm a_0 \right)}{2} \sqrt[2]{\frac{1}{\left((Z-11) - \left(\frac{1}{8} - \frac{3}{Z} \right) \frac{\sqrt{3}}{r_{10}} \right)} + \frac{20\sqrt{3} \left(\left[\frac{Z-12}{Z-11} \right] \left(1 + \frac{\sqrt{2}}{2} \right) r_{10} \right)}{\left((Z-11) - \left(\frac{1}{8} - \frac{3}{Z} \right) \frac{\sqrt{3}}{r_{10}} \right)}} \quad (68)$$

r_{10} in units of a_0

where r_{10} is given by Eq. (67) (Eq. (10.212)), and $n-12$ electrons in a 3p orbitsphere with radius r_n given by

$$r_n = \frac{\left(\frac{a_0}{\left((Z-(n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right)} \pm a_0 \right)}{2} \sqrt[2]{\frac{1}{\left((Z-(n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right)} + \frac{20\sqrt{3} \left(\left[\frac{Z-n}{Z-(n-1)} \right] \left(1 - \frac{\sqrt{2}}{2} + \frac{1}{2} \right) r_{12} \right)}{\left((Z-(n-1)) - \left(\frac{A}{8} - \frac{B}{2Z} \right) \frac{\sqrt{3}}{r_{12}} \right)}} \quad (69)$$

r_{12} in units of a_0

10 where r_{12} is given by Eq. (68) (Eqs. (10.255) and (10.404)), the parameter A given

in TABLE XXIII corresponds to the diamagnetic force, $F_{\text{diamagnetic}}$, (Eq. (10.258)), and the parameter B given in TABLE XXIII corresponds to the paramagnetic force, F_{mag} (Eqs. (10.260-10.264)). The positive root of Eq. (69) must be taken in order that $r_n > 0$. The radii of several n-electron 3p atoms are given in TABLES XIII-XVIII.

5 The ionization energy for the aluminum atom is given by Eq. (10.227). The ionization energies for the n-electron 3p atoms are given by the negative of the electric energy, $E(\text{electric})$, (Eq. (61) with the radii, r_n , given by Eq. (69)). Since the relativistic corrections were small, the nonrelativistic ionization energies for experimentally measured n-electron 3p atoms are given by Eqs. (61) and (69) in
10 TABLES XIII-XVIII.

Systems

Embodiments of the system for performing computing and rendering of the
15 nature atomic and atomic-ionic electrons using the physical solutions may comprise a general purpose computer. Such a general purpose computer may have any number of basic configurations. For example, such a general purpose computer may comprise a central processing unit (CPU), one or more specialized processors, system memory, a mass storage device such as a magnetic disk, an optical disk, or
20 other storage device, an input means such as a keyboard or mouse, a display device, and a printer or other output device. A system implementing the present invention can also comprise a special purpose computer or other hardware system and all should be included within its scope.

The display can be static or dynamic such that spin and angular motion with
25 corresponding momenta can be displayed in an embodiment. The displayed information is useful to anticipate reactivity and physical properties. The insight into the nature of atomic and atomic-ionic electrons can permit the solution and display of other atoms and atomic ions and provide utility to anticipate their reactivity and physical properties. Furthermore, the displayed information is useful in teaching
30 environments to teach students the properties of electrons.

Embodiments within the scope of the present invention also include computer program products comprising computer readable medium having embodied therein program code means. Such computer readable media can be any available media which can be accessed by a general purpose or special purpose computer. By way
35 of example, and not limitation, such computer readable media can comprise RAM,

ROM, EPROM, CD ROM, DVD or other optical disk storage, magnetic disk storage or other magnetic storage devices, or any other medium which can embody the desired program code means and which can be accessed by a general purpose or special purpose computer. Combinations of the above should also be included within the scope of computer readable media. Program code means comprises, for example, executable instructions and data which cause a general purpose computer or special purpose computer to perform a certain function of a group of functions.

A specific example of the rendering of the electron of atomic hydrogen using Mathematica and computed on a PC is shown in FIGURE 1. The algorithm used was

To generate a spherical shell:

SphericalPlot3D[1,{q,0,p},{f,0,2p},Boxed@False,Axes@False];. The rendering can be viewed from different perspectives. A specific example of the rendering of atomic hydrogen using Mathematica and computed on a PC is shown in FIGURE 1. The algorithm used was

To generate the picture of the electron and proton:

```
Electron=SphericalPlot3D[1,{q,0,p},{f,0,2p-p/2},Boxed@False,Axes@False];
Proton=Show[Graphics3D[{Blue,PointSize[0.03],Point[{0,0,0}]}],Boxed@False];
Show[Electron,Proton];
```

Specific examples of the rendering of the spherical-and-time-harmonic-electron-charge-density functions using Mathematica and computed on a PC are shown in FIGURE 3. The algorithm used was

To generate L1MO:

```
L1MOcolors[theta_,phi_,det_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det
<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.533
3,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,RGB
Color[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RGB
Color[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColor[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.075,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.326,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];
```

```
L1MO=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]
Sin[phi],Cos[theta],L1MOcolors[theta,phi,1+Cos[theta]]},{theta,0,Pi},{phi,0,2Pi},Boxe
d@False,Axes@False,Lighting@False,PlotPoints@{20,20},ViewPoint@{-0.273,-
2.030,3.494}];
```

5

To generate L1MX:

```
L1MXcolors[theta_, phi_, det_] = Which[det < 0.1333, RGBColor[1.000, 0.070,
0.079],det < .2666, RGBColor[1.000, 0.369, 0.067],det < .4, RGBColor[1.000, 0.681,
10 0.049],det < .5333, RGBColor[0.984, 1.000, 0.051], det < .6666, RGBColor[0.673,
1.000, 0.058], det < .8, RGBColor[0.364, 1.000, 0.055],det < .9333,
RGBColor[0.071, 1.000, 0.060], det < 1.066, RGBColor[0.085, 1.000, 0.388],det <
1.2, RGBColor[0.070, 1.000, 0.678], det < 1.333, RGBColor[0.070, 1.000,
1.000],det < 1.466, RGBColor[0.067, 0.698, 1.000], det < 1.6, RGBColor[0.075,
15 0.401, 1.000],det < 1.733, RGBColor[0.067, 0.082, 1.000], det < 1.866,
RGBColor[0.326, 0.056, 1.000],det <= 2, RGBColor[0.674, 0.079, 1.000]];
```

```
L1MX=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]
Sin[phi],Cos[theta],L1MXcolors[theta,phi,1+Sin[theta]
20 Cos[phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed@False,Axes@False,Lighting@False,PlotPoin
ts@{20,20},ViewPoint@{-0.273,-2.030,3.494}];
```

To generate L1MY:

```
25 L1MYcolors[theta_,phi_,det_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],det
<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.533
3,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,RG
BColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RGB
Color[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBColo
30 r[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0.0
75,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.32
6,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];
```

```
L1MY=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]
35 Sin[phi],Cos[theta],L1MYcolors[theta,phi,1+Sin[theta]
Sin[phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed@False,Axes@False,Lighting@False,PlotPoint
```


s@{20,20});

To generate L2MO:

```

5  L2MOcolors[theta_, phi_, det_] = Which[det < 0.2, RGBColor[1.000, 0.070,
    0.079], det < .4, RGBColor[1.000, 0.369, 0.067], det < .6, RGBColor[1.000, 0.681,
    0.049], det < .8, RGBColor[0.984, 1.000, 0.051], det < 1, RGBColor[0.673, 1.000,
    0.058], det < 1.2, RGBColor[0.364, 1.000, 0.055], det < 1.4, RGBColor[0.071, 1.000,
    0.060], det < 1.6, RGBColor[0.085, 1.000, 0.388], det < 1.8, RGBColor[0.070, 1.000,
10 0.678], det < 2, RGBColor[0.070, 1.000, 1.000], det < 2.2, RGBColor[0.067, 0.698,
    1.000], det < 2.4, RGBColor[0.075, 0.401, 1.000], det < 2.6, RGBColor[0.067, 0.082,
    1.000], det < 2.8, RGBColor[0.326, 0.056, 1.000], det <= 3, RGBColor[0.674, 0.079,
    1.000]];

15 L2MO=ParametricPlot3D[{Sin[theta] Cos[phi], Sin[theta] Sin[phi], Cos[theta],
    L2MOcolors[theta, phi, 3Cos[theta] Cos[theta]]},
    {theta, 0, Pi}, {phi, 0, 2Pi},
    Boxed -> False, Axes -> False, Lighting -> False,
    PlotPoints-> {20, 20},
20  ViewPoint->{-0.273, -2.030, 3.494}];

```

To generate L2MF:

```

L2MFcolors[theta_, phi_, det_] = Which[det < 0.1333, RGBColor[1.000, 0.070, 0.079], det <
25 .2666, RGBColor[1.000, 0.369, 0.067], det < .4, RGBColor[1.000, 0.681, 0.049], det < .5333,
    RGBColor[0.984, 1.000, 0.051], det < .6666, RGBColor[0.673, 1.000, 0.058], det < .8, RGB
    Color[0.364, 1.000, 0.055], det < .9333, RGBColor[0.071, 1.000, 0.060], det < 1.066, RGB
    Color[0.085, 1.000, 0.388], det < 1.2, RGBColor[0.070, 1.000, 0.678], det < 1.333, RGB
    Color[0.070, 1.000, 1.000], det < 1.466, RGBColor[0.067, 0.698, 1.000], det < 1.6, RGBColor[0.07
30 5, 0.401, 1.000], det < 1.733, RGBColor[0.067, 0.082, 1.000], det < 1.866, RGBColor[0.326,
    0.056, 1.000], det < 2, RGBColor[0.674, 0.079, 1.000]];

L2MF=ParametricPlot3D[{Sin[theta] Cos[phi], Sin[theta]
    Sin[phi], Cos[theta], L2MFcolors[theta, phi, 1+.72618 Sin[theta] Cos[phi] 5 Cos[theta]
35 Cos[theta] -.72618 Sin[theta]
    Cos[phi]]}, {theta, 0, Pi}, {phi, 0, 2Pi}, Boxed@False, Axes@False, Lighting@False, PlotPoin

```

ts@{20,20},ViewPoint@{-0.273,-2.030,2.494}};

To generate L2MX2Y2:

5 L2MX2Y2colors[theta_,phi_,det_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],
det<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.
5333,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,
RGBColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,R
GBColor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGB
10 Color[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColo
r[0.075,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[
0.326,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];

L2MX2Y2=ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]
15 Sin[phi],Cos[theta],L2MX2Y2colors[theta,phi,1+Sin[theta] Sin[theta] Cos[2
phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed@False,Axes@False,Lighting@False,PlotPoints@{
20,20},ViewPoint@{-0.273,-2.030,3.494}};

To generate L2MXY:

20 L2MXYcolors[theta_,phi_,det_]=Which[det<0.1333,RGBColor[1.000,0.070,0.079],de
t<.2666,RGBColor[1.000,0.369,0.067],det<.4,RGBColor[1.000,0.681,0.049],det<.53
33,RGBColor[0.984,1.000,0.051],det<.6666,RGBColor[0.673,1.000,0.058],det<.8,R
GBColor[0.364,1.000,0.055],det<.9333,RGBColor[0.071,1.000,0.060],det<1.066,RG
25 BColor[0.085,1.000,0.388],det<1.2,RGBColor[0.070,1.000,0.678],det<1.333,RGBCo
lor[0.070,1.000,1.000],det<1.466,RGBColor[0.067,0.698,1.000],det<1.6,RGBColor[0
.075,0.401,1.000],det<1.733,RGBColor[0.067,0.082,1.000],det<1.866,RGBColor[0.3
26,0.056,1.000],det£2,RGBColor[0.674,0.079,1.000]];

30 ParametricPlot3D[{Sin[theta] Cos[phi],Sin[theta]
Sin[phi],Cos[theta],L2MXYcolors[theta,phi,1+Sin[theta] Sin[theta] Sin[2
phi]]},{theta,0,Pi},{phi,0,2Pi},Boxed@False,Axes@False,Lighting@False,PlotPoints@{
20,20},ViewPoint@{-0.273,-2.030,3.494}};

35 The present invention may be embodied in other specific forms without
departing from the spirit or essential attributes thereof and, accordingly, reference
should be made to the appended claims, rather than to the foregoing specification,

as indicating the scope of the invention.

The following list of references are incorporated by reference in their entirety and referred to throughout this application by use of brackets.

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